乙二醇作为反应物的反应表19-4

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: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.60924 HOMO: -6.91169 LUMO: -0.53879 factor:1 | 1 (-0.37895) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.65613 HOMO: -7.29809 LUMO: 2.83543 factor:1 | -1 (0.57416) | 1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.60634 HOMO: -6.86543 LUMO: -0.70205 factor:1 | -1 (0.62396) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.71619 HOMO: -7.47769 LUMO: 0.31293 factor:1 | -1 (0.51410) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.34926 HOMO: -6.63141 LUMO: -0.55511 factor:1 | 1 (-0.11897) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.41553 HOMO: -6.68856 LUMO: -0.30205 factor:1 | -1 (0.81476) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.24826 HOMO: -7.22190 LUMO: 0.53334 factor:1 | -1 (0.98203) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.49115 HOMO: -6.66407 LUMO: -0.27756 factor:1 | -1 (0.73914) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.65173 HOMO: -7.15659 LUMO: -0.70205 factor:1 | -1 (0.57857) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.90787 HOMO: -6.69400 LUMO: 1.67622 factor:1 | -1 (0.32243) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.81431 HOMO: -6.60420 LUMO: 2.16058 factor:1 | -1 (0.41598) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.43955 HOMO: -6.87087 LUMO: 1.88031 factor:1 | 1 (-0.20926) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.97309 HOMO: -6.60965 LUMO: -0.19864 factor:1 | -1 (0.25720) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.76933 HOMO: -7.29265 LUMO: 0.52246 factor:1 | -1 (0.46096) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.45281 HOMO: -6.86543 LUMO: -0.59593 factor:1 | -1 (0.77748) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.54781 HOMO: -7.44504 LUMO: -1.01226 factor:1 | -1 (0.68249) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.41180 HOMO: -6.92530 LUMO: -0.75103 factor:1 | -1 (0.81849) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.63627 HOMO: -7.10489 LUMO: 2.20412 factor:1 | -1 (0.59402) | 1 | 1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.59573 HOMO: -6.58788 LUMO: 1.73881 factor:1 | -1 (0.63457) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.73935 HOMO: -6.64502 LUMO: 1.70343 factor:1 | -1 (0.49095) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.16050 HOMO: -6.73754 LUMO: 1.60819 factor:1 | -1 (0.06980) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.59520 HOMO: -6.80829 LUMO: 2.45991 factor:1 | 1 (-0.36490) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.06536 HOMO: -6.91713 LUMO: 2.43814 factor:1 | 1 (-0.83506) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.45601 HOMO: -6.60692 LUMO: 1.93745 factor:1 | 1 (-0.22572) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.46673 HOMO: -6.26134 LUMO: 1.46125 factor:1 | 1 (-0.23644) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.06792 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-0.83762) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.76654 HOMO: -6.97700 LUMO: -0.73471 factor:1 | 1 (-1.53625) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.51235 HOMO: -6.92258 LUMO: -0.70205 factor:1 | -1 (0.71795) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.64184 HOMO: -6.83550 LUMO: -0.56872 factor:1 | 1 (-0.41155) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.89940 HOMO: -6.72121 LUMO: 1.89663 factor:1 | 1 (-0.66910) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.75738 HOMO: -6.73482 LUMO: 1.89935 factor:1 | 1 (-0.52708) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.12359 HOMO: -6.61781 LUMO: 1.86670 factor:1 | 1 (-0.89330) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.65166 HOMO: -7.01782 LUMO: 2.26399 factor:1 | 1 (-0.42137) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.29543 HOMO: -7.23551 LUMO: 2.09800 factor:1 | 1 (-1.06514) | 1 | 1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.49222 HOMO: -7.13483 LUMO: 2.17963 factor:1 | 1 (-1.26193) | 1 | 1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.93632 HOMO: -6.22869 LUMO: 2.01092 factor:1 | 1 (-0.70603) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.27733 HOMO: -6.80285 LUMO: 2.14970 factor:1 | -1 (0.95297) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.30535 HOMO: -7.21102 LUMO: 2.33746 factor:1 | -1 (0.92494) | 1 | 1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.49376 HOMO: -6.39740 LUMO: 2.59597 factor:1 | -1 (0.73653) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.74166 HOMO: -7.07768 LUMO: 2.48168 factor:1 | -1 (0.48863) | 1 | 1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.45967 HOMO: -7.11306 LUMO: 0.90614 factor:1 | -1 (0.77063) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.37950 HOMO: -6.61781 LUMO: -2.46263 factor:1 | -1 (0.85079) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.25047 HOMO: -6.96611 LUMO: 0.90614 factor:1 | -1 (0.97983) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.40574 HOMO: -6.86271 LUMO: -1.14832 factor:1 | -1 (0.82456) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.89937 HOMO: -6.72665 LUMO: 0.96873 factor:1 | 1 (-0.66907) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.63946 HOMO: -7.14571 LUMO: 1.05036 factor:1 | 1 (-1.40917) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.91014 HOMO: -7.14299 LUMO: 0.98777 factor:1 | 1 (-0.67985) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.94982 HOMO: -6.99333 LUMO: 1.05852 factor:1 | 1 (-0.71952) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.40753 HOMO: -6.78924 LUMO: -1.49935 factor:1 | -1 (0.82276) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.53783 HOMO: -7.13755 LUMO: 0.94151 factor:1 | -1 (1.69247) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.89415 HOMO: -6.72938 LUMO: -0.35375 factor:1 | -1 (0.33614) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.50693 HOMO: -6.99061 LUMO: 0.82450 factor:1 | -1 (0.72336) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.58332 HOMO: -6.75114 LUMO: -0.68028 factor:1 | -1 (0.64698) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.30865 HOMO: -6.40556 LUMO: -0.42722 factor:1 | -1 (0.92165) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.53289 HOMO: -7.18653 LUMO: 0.42178 factor:1 | -1 (0.69740) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.23647 HOMO: -6.63958 LUMO: -0.71294 factor:1 | -1 (2.99382) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.07339 HOMO: -6.63958 LUMO: -0.71022 factor:1 | -1 (0.15690) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.85646 HOMO: -6.69672 LUMO: -0.72654 factor:1 | -1 (0.37383) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.43960 HOMO: -6.56883 LUMO: -0.80274 factor:1 | 1 (-0.20931) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.07034 HOMO: -6.68584 LUMO: -0.56872 factor:1 | 1 (-0.84004) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.43569 HOMO: -6.59060 LUMO: -0.35647 factor:1 | 1 (-0.20539) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.21664 HOMO: -6.72121 LUMO: -0.71838 factor:1 | -1 (1.01365) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.24002 HOMO: -6.57971 LUMO: -0.61498 factor:1 | -1 (0.99028) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.85029 HOMO: -7.07496 LUMO: 0.50613 factor:1 | -1 (0.38001) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.24442 HOMO: -7.14027 LUMO: 0.43266 factor:1 | 1 (-0.01412) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.28385 HOMO: -6.43277 LUMO: -0.44082 factor:1 | -1 (2.94645) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.98486 HOMO: -6.79468 LUMO: 0.07619 factor:1 | -1 (1.24544) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.92592 HOMO: -6.81917 LUMO: -2.57148 factor:1 | -1 (1.30438) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.12716 HOMO: -6.71849 LUMO: 1.30615 factor:1 | -1 (0.10313) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.06368 HOMO: -6.85455 LUMO: -0.63675 factor:1 | -1 (0.16662) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.59322 HOMO: -6.73210 LUMO: -1.03131 factor:1 | -1 (0.63707) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.75031 HOMO: -6.83550 LUMO: -0.58777 factor:1 | -1 (0.47998) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.86817 HOMO: -6.53073 LUMO: -0.74287 factor:1 | -1 (0.36213) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.61154 HOMO: -7.18381 LUMO: -0.92791 factor:1 | -1 (0.61876) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.43561 HOMO: -6.49264 LUMO: -0.44627 factor:1 | -1 (0.79468) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.47172 HOMO: -7.32803 LUMO: 0.41361 factor:1 | -1 (0.75857) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.64727 HOMO: -6.53073 LUMO: -0.52790 factor:1 | -1 (1.58302) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.04613 HOMO: -6.54978 LUMO: -0.53062 factor:1 | -1 (0.18417) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.95560 HOMO: -6.56611 LUMO: -0.37824 factor:1 | -1 (0.27470) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.17700 HOMO: -6.57155 LUMO: -0.64219 factor:1 | -1 (1.05330) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.09797 HOMO: -7.08040 LUMO: 0.45715 factor:1 | -1 (0.13233) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.36108 HOMO: -6.66679 LUMO: -0.75376 factor:1 | -1 (0.86921) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.44691 HOMO: -6.83550 LUMO: -0.99322 factor:1 | -1 (0.78339) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.84754 HOMO: -6.53345 LUMO: -0.29660 factor:1 | -1 (0.38276) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.81399 HOMO: -6.65046 LUMO: 2.40549 factor:1 | -1 (0.41631) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.70977 HOMO: -6.98788 LUMO: 2.01092 factor:1 | -1 (0.52053) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.41242 HOMO: -6.61781 LUMO: 1.92384 factor:1 | 1 (-0.18213) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.42337 HOMO: -6.61237 LUMO: 2.06807 factor:1 | -1 (0.80693) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.30758 HOMO: -6.59060 LUMO: 1.95106 factor:1 | -1 (0.92271) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.03727 HOMO: -6.48175 LUMO: 1.72248 factor:1 | -1 (1.19303) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.87095 HOMO: -6.84911 LUMO: 2.03541 factor:1 | -1 (1.35934) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.01298 HOMO: -6.50624 LUMO: 2.17147 factor:1 | 1 (-0.78268) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.01231 HOMO: -6.68312 LUMO: 2.08439 factor:1 | -1 (1.21798) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.18094 HOMO: -6.96067 LUMO: 1.98099 factor:1 | -1 (1.04935) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.34257 HOMO: -6.93618 LUMO: 1.85854 factor:1 | 1 (-0.11227) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.40009 HOMO: -6.71305 LUMO: -0.61226 factor:1 | 1 (-0.16980) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.93986 HOMO: -7.06408 LUMO: 0.80001 factor:1 | 1 (-0.70956) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.98468 HOMO: -6.52257 LUMO: 0.99049 factor:1 | -1 (0.24561) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.14836 HOMO: -6.84638 LUMO: 1.10750 factor:1 | -1 (0.08193) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.95734 HOMO: -6.85455 LUMO: 0.84900 factor:1 | -1 (0.27296) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.96158 HOMO: -6.60148 LUMO: -0.78369 factor:1 | -1 (0.26871) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.06177 HOMO: -6.86543 LUMO: -0.93063 factor:1 | -1 (0.16852) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.63756 HOMO: -6.70489 LUMO: -0.72382 factor:1 | -1 (1.59274) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.58234 HOMO: -6.59060 LUMO: 0.31293 factor:1 | -1 (0.64796) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.93402 HOMO: -6.52257 LUMO: -0.48708 factor:1 | -1 (0.29628) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.87914 HOMO: -6.54706 LUMO: -0.48164 factor:1 | -1 (1.35115) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.95584 HOMO: -7.32803 LUMO: 0.08436 factor:1 | -1 (0.27445) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.79516 HOMO: -6.77291 LUMO: -0.66940 factor:1 | -1 (0.43514) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.50435 HOMO: -6.68312 LUMO: -0.53062 factor:1 | -1 (0.72595) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.12183 HOMO: -7.07768 LUMO: 0.45987 factor:1 | -1 (0.10846) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.34846 HOMO: -6.50352 LUMO: -0.63675 factor:1 | -1 (0.88184) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.86047 HOMO: -6.48992 LUMO: -0.60681 factor:1 | -1 (0.36983) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.46097 HOMO: -6.65318 LUMO: -0.72382 factor:1 | -1 (0.76932) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.54390 HOMO: -6.54706 LUMO: 0.24218 factor:1 | -1 (1.68640) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.82180 HOMO: -6.63958 LUMO: 0.57416 factor:1 | -1 (0.40850) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.18991 HOMO: -6.37563 LUMO: -0.48164 factor:1 | -1 (0.04038) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.94196 HOMO: -6.64774 LUMO: -0.71838 factor:1 | -1 (0.28833) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.84199 HOMO: -7.17020 LUMO: 0.45987 factor:1 | -1 (0.38831) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.86655 HOMO: -6.86543 LUMO: -1.05036 factor:1 | 1 (-0.63626) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.73531 HOMO: -6.77019 LUMO: -1.03131 factor:1 | 1 (-0.50502) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.41762 HOMO: -6.80285 LUMO: 1.05852 factor:1 | 1 (-0.18732) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.93082 HOMO: -6.76475 LUMO: 1.01771 factor:1 | 1 (-0.70053) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.58087 HOMO: -6.92530 LUMO: 1.37417 factor:1 | -1 (0.64943) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.96947 HOMO: -6.98244 LUMO: 1.25989 factor:1 | -1 (0.26082) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.05260 HOMO: -6.74842 LUMO: 0.89798 factor:1 | -1 (0.17769) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.15174 HOMO: -6.77019 LUMO: -1.17009 factor:1 | -1 (0.07856) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.00245 HOMO: -6.78652 LUMO: 1.35785 factor:1 | -1 (0.22784) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.86403 HOMO: -6.82734 LUMO: -0.68301 factor:1 | -1 (0.36627) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.65306 HOMO: -6.48175 LUMO: -2.19052 factor:1 | -1 (0.57724) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.65894 HOMO: -6.65863 LUMO: -0.77008 factor:1 | -1 (0.57136) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.43906 HOMO: -6.44094 LUMO: -2.20956 factor:1 | 1 (-0.20877) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.73399 HOMO: -6.59876 LUMO: -0.57688 factor:1 | -1 (0.49631) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.60743 HOMO: -6.78380 LUMO: -0.77008 factor:1 | -1 (0.62287) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.04612 HOMO: -7.30354 LUMO: 0.25034 factor:1 | 1 (-0.81582) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.61954 HOMO: -6.59332 LUMO: -0.53334 factor:1 | -1 (0.61076) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.38692 HOMO: -6.64230 LUMO: -0.55783 factor:1 | 1 (-0.15663) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.33519 HOMO: -7.26544 LUMO: 0.20409 factor:1 | 1 (-0.10490) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.80841 HOMO: -6.61237 LUMO: -0.65307 factor:1 | -1 (0.42189) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.72272 HOMO: -6.72393 LUMO: -0.65307 factor:1 | -1 (0.50757) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.43384 HOMO: -6.29671 LUMO: -0.39729 factor:1 | -1 (0.79645) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.54245 HOMO: -6.75387 LUMO: -0.53334 factor:1 | -1 (0.68785) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.39013 HOMO: -6.53073 LUMO: -0.31293 factor:1 | 1 (-0.15984) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.58460 HOMO: -6.42189 LUMO: -0.59049 factor:1 | -1 (0.64570) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.34045 HOMO: -6.41100 LUMO: -0.29933 factor:1 | 1 (-0.11015) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.71063 HOMO: -6.57427 LUMO: -0.53879 factor:1 | 1 (-0.48034) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.37660 HOMO: -7.43143 LUMO: 0.33470 factor:1 | 1 (-1.14631) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.20442 HOMO: -6.56067 LUMO: -0.50885 factor:1 | -1 (0.02588) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.40325 HOMO: -6.65863 LUMO: -0.76464 factor:1 | 1 (-0.17296) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.97156 HOMO: -6.32665 LUMO: -0.41906 factor:1 | 1 (-0.74127) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.50037 HOMO: -6.57699 LUMO: 1.63813 factor:1 | 1 (-0.27007) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.68176 HOMO: -6.53073 LUMO: 1.71704 factor:1 | 1 (-0.45146) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.08906 HOMO: -6.86271 LUMO: 2.07351 factor:1 | 1 (-0.85876) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.45860 HOMO: -6.63686 LUMO: 1.78235 factor:1 | 1 (-0.22830) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.99009 HOMO: -6.60965 LUMO: 1.94289 factor:1 | 1 (-0.75980) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.34388 HOMO: -6.55250 LUMO: 1.89119 factor:1 | 1 (-0.11358) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.42087 HOMO: -6.50624 LUMO: 1.85582 factor:1 | -1 (0.80943) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.97428 HOMO: -6.06814 LUMO: 1.94561 factor:1 | 1 (-0.74399) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.53718 HOMO: -6.58788 LUMO: 2.01908 factor:1 | 1 (-0.30689) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.09969 HOMO: -6.74026 LUMO: 0.31293 factor:1 | -1 (1.13061) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.55261 HOMO: -6.54434 LUMO: -0.42994 factor:1 | 1 (-0.32232) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.09209 HOMO: -6.94707 LUMO: 0.42994 factor:1 | -1 (0.13821) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.36595 HOMO: -6.98516 LUMO: 0.41361 factor:1 | -1 (0.86434) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.31794 HOMO: -6.31304 LUMO: -0.54967 factor:1 | 1 (-0.08765) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.91257 HOMO: -6.48447 LUMO: -0.40817 factor:1 | 1 (-0.68227) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.75773 HOMO: -6.49264 LUMO: 0.29116 factor:1 | 1 (-0.52744) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.88769 HOMO: -6.48719 LUMO: -0.11973 factor:1 | 1 (-1.65739) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.94038 HOMO: -7.16204 LUMO: 0.44082 factor:1 | -1 (0.28991) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.01480 HOMO: -6.74842 LUMO: -0.37552 factor:1 | 1 (-0.78450) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.86707 HOMO: -6.44638 LUMO: -0.45171 factor:1 | 1 (-0.63677) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.22436 HOMO: -7.07496 LUMO: 0.50341 factor:1 | -1 (0.00593) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.82591 HOMO: -6.79468 LUMO: 0.11429 factor:1 | -1 (0.40439) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.84666 HOMO: -6.63958 LUMO: -0.67484 factor:1 | 1 (-0.61637) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.26374 HOMO: -7.08584 LUMO: 0.46259 factor:1 | 1 (-0.03344) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.90719 HOMO: -6.80285 LUMO: -0.73199 factor:1 | -1 (0.32311) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.62058 HOMO: -6.44366 LUMO: -0.45443 factor:1 | 1 (-1.39028) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.75425 HOMO: -6.75931 LUMO: 0.25851 factor:1 | 1 (-0.52396) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.17586 HOMO: -6.64502 LUMO: 1.79323 factor:1 | 1 (-0.94557) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.50848 HOMO: -6.51168 LUMO: 1.60275 factor:1 | 1 (-0.27818) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.28684 HOMO: -6.56067 LUMO: 1.63268 factor:1 | 1 (-0.05655) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.87091 HOMO: -6.56883 LUMO: 1.70615 factor:1 | -1 (0.35938) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.09750 HOMO: -6.77836 LUMO: 1.77962 factor:1 | -1 (0.13279) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.85061 HOMO: -6.38923 LUMO: 1.85854 factor:1 | 1 (-0.62031) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.53944 HOMO: -6.35658 LUMO: 2.16875 factor:1 | 1 (-0.30915) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.46743 HOMO: -6.83006 LUMO: 2.31025 factor:1 | 1 (-1.23714) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.83100 HOMO: -6.87087 LUMO: 1.79051 factor:1 | 1 (-1.60071) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.37660 HOMO: -6.56339 LUMO: 2.37828 factor:1 | 1 (-1.14631) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.93999 HOMO: -6.30488 LUMO: 2.51705 factor:1 | 1 (-1.70969) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.78208 HOMO: -6.69400 LUMO: 1.95650 factor:1 | 1 (-1.55178) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.26814 HOMO: -6.51168 LUMO: 2.03541 factor:1 | 1 (-1.03784) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.11703 HOMO: -6.30760 LUMO: 1.65173 factor:1 | 1 (-0.88674) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.33829 HOMO: -6.55250 LUMO: 1.90752 factor:1 | 1 (-1.10799) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.24855 HOMO: -6.41372 LUMO: 1.76058 factor:1 | 1 (-1.01825) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.48407 HOMO: -6.23957 LUMO: 2.06534 factor:1 | 1 (-0.25377) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.43525 HOMO: -6.58243 LUMO: 2.11705 factor:1 | 1 (-0.20496) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.63675 HOMO: -6.37835 LUMO: 2.09256 factor:1 | 1 (-0.40646) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.08607 HOMO: -6.50624 LUMO: 2.55787 factor:1 | 1 (-0.85577) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.24640 HOMO: -6.45454 LUMO: 1.87214 factor:1 | 1 (-1.01610) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.64029 HOMO: -6.53617 LUMO: 1.95650 factor:1 | 1 (-0.40999) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.24050 HOMO: -6.51985 LUMO: 1.71432 factor:1 | 1 (-0.01020) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.38094 HOMO: -6.75114 LUMO: 1.84493 factor:1 | 1 (-0.15064) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.59122 HOMO: -6.06270 LUMO: 1.65717 factor:1 | 1 (-1.36092) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.48957 HOMO: -5.89671 LUMO: 1.71704 factor:1 | 1 (-0.25927) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.10400 HOMO: -6.18787 LUMO: 1.91840 factor:1 | 1 (-0.87370) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.70606 HOMO: -6.01644 LUMO: 1.85582 factor:1 | 1 (-0.47576) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.87353 HOMO: -6.05998 LUMO: 2.33474 factor:1 | -1 (0.35677) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.84372 HOMO: -6.05725 LUMO: 2.03541 factor:1 | 1 (-0.61343) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.52930 HOMO: -6.80829 LUMO: 1.90480 factor:1 | -1 (0.70099) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.23852 HOMO: -6.76475 LUMO: 2.20956 factor:1 | -1 (0.99177) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.33861 HOMO: -6.29944 LUMO: 1.77962 factor:1 | -1 (0.89169) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.51624 HOMO: -6.47359 LUMO: -0.25579 factor:1 | -1 (0.71405) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.76348 HOMO: -6.57699 LUMO: -0.47348 factor:1 | -1 (0.46681) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.31261 HOMO: -7.20830 LUMO: 0.49797 factor:1 | 1 (-0.08231) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.52579 HOMO: -7.49402 LUMO: 0.29933 factor:1 | -1 (0.70450) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.60797 HOMO: -6.66679 LUMO: -0.58777 factor:1 | -1 (0.62232) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.36767 HOMO: -6.67767 LUMO: -0.56328 factor:1 | -1 (0.86263) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.40086 HOMO: -7.42871 LUMO: 0.35647 factor:1 | -1 (0.82943) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.71110 HOMO: -6.56067 LUMO: -0.54423 factor:1 | -1 (0.51919) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.67736 HOMO: -6.56339 LUMO: -0.50341 factor:1 | -1 (0.55294) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.43482 HOMO: -6.56067 LUMO: -0.48436 factor:1 | 1 (-0.20452) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.08803 HOMO: -6.73210 LUMO: 1.75241 factor:1 | -1 (0.14226) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.89558 HOMO: -6.48175 LUMO: 1.91296 factor:1 | 1 (-1.66528) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.81588 HOMO: -6.67767 LUMO: 1.70343 factor:1 | 1 (-0.58559) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.27081 HOMO: -6.37835 LUMO: 1.96466 factor:1 | 1 (-0.04052) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.58685 HOMO: -6.40828 LUMO: 2.10072 factor:1 | 1 (-0.35655) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.28238 HOMO: -6.06542 LUMO: 1.92112 factor:1 | 1 (-0.05208) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.90226 HOMO: -6.90353 LUMO: 1.83133 factor:1 | -1 (0.32803) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.67053 HOMO: -6.37019 LUMO: 1.92929 factor:1 | -1 (0.55977) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.00769 HOMO: -6.61509 LUMO: 2.11160 factor:1 | -1 (1.22261) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.15955 HOMO: -6.82734 LUMO: 1.77146 factor:1 | -1 (1.07074) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.62819 HOMO: -6.01100 LUMO: 1.89935 factor:1 | -1 (0.60211) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.48647 HOMO: -6.49536 LUMO: 1.75241 factor:1 | -1 (0.74382) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.87608 HOMO: -6.34297 LUMO: 1.86398 factor:1 | -1 (0.35421) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.76185 HOMO: -6.53073 LUMO: 1.84493 factor:1 | -1 (0.46844) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.97182 HOMO: -6.53345 LUMO: 2.41093 factor:1 | -1 (1.25847) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.04347 HOMO: -7.01237 LUMO: 2.06262 factor:1 | -1 (1.18682) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.30562 HOMO: -6.17154 LUMO: 1.89119 factor:1 | -1 (0.92467) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.08831 HOMO: -6.08719 LUMO: 1.74425 factor:1 | -1 (1.14198) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.73761 HOMO: -6.69672 LUMO: 1.95106 factor:1 | -1 (0.49269) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.56038 HOMO: -6.58243 LUMO: 2.24766 factor:1 | -1 (0.66992) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.41828 HOMO: -6.74570 LUMO: 2.02181 factor:1 | -1 (0.81201) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.54963 HOMO: -6.53890 LUMO: 1.92929 factor:1 | -1 (0.68067) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.63306 HOMO: -6.03276 LUMO: 1.67078 factor:1 | -1 (0.59724) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.99919 HOMO: -6.67767 LUMO: 2.03541 factor:1 | -1 (0.23111) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.82221 HOMO: -5.98378 LUMO: 1.84221 factor:1 | -1 (0.40809) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.57491 HOMO: -6.07086 LUMO: 2.01908 factor:1 | -1 (0.65539) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.47395 HOMO: -6.29944 LUMO: 1.90208 factor:1 | 1 (-0.24365) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.76035 HOMO: -6.75114 LUMO: 1.85854 factor:1 | 1 (-0.53005) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.89186 HOMO: -6.56611 LUMO: 2.49801 factor:1 | 1 (-0.66156) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.05636 HOMO: -6.39740 LUMO: 1.92929 factor:1 | -1 (0.17394) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.24665 HOMO: -6.85999 LUMO: -1.07757 factor:1 | 1 (-0.01635) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.87926 HOMO: -6.98244 LUMO: 1.07213 factor:1 | 1 (-0.64896) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.45876 HOMO: -7.04231 LUMO: 0.64219 factor:1 | 1 (-0.22847) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.56064 HOMO: -6.96339 LUMO: 0.75648 factor:1 | 1 (-0.33035) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.79347 HOMO: -6.83822 LUMO: -0.97417 factor:1 | -1 (0.43682) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.14157 HOMO: -6.44910 LUMO: -2.15242 factor:1 | -1 (1.08873) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.06570 HOMO: -6.84094 LUMO: -1.37690 factor:1 | -1 (1.16459) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.02172 HOMO: -6.74026 LUMO: -2.54699 factor:1 | -1 (0.20858) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.39547 HOMO: -6.96611 LUMO: 1.24900 factor:1 | 1 (-0.16517) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.77112 HOMO: -7.21102 LUMO: 0.82995 factor:1 | 1 (-0.54083) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.09309 HOMO: -6.88448 LUMO: 0.81634 factor:1 | 1 (-0.86279) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.98160 HOMO: -7.04231 LUMO: 1.10750 factor:1 | 1 (-0.75131) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.56611 HOMO: -6.83550 LUMO: -0.98777 factor:1 | 1 (-0.33582) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.35046 HOMO: -6.82189 LUMO: 0.93879 factor:1 | 1 (-0.12017) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.21644 HOMO: -6.81101 LUMO: 0.70750 factor:1 | 1 (-0.98614) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.97308 HOMO: -7.06680 LUMO: 0.74015 factor:1 | 1 (-1.74278) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.95063 HOMO: -6.68856 LUMO: 0.86260 factor:1 | 1 (-0.72034) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.15963 HOMO: -6.83822 LUMO: -0.63403 factor:1 | -1 (0.07067) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.16189 HOMO: -6.84911 LUMO: 1.26533 factor:1 | -1 (0.06841) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.28834 HOMO: -7.01237 LUMO: 0.73743 factor:1 | 1 (-0.05804) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.73839 HOMO: -7.00965 LUMO: 1.40139 factor:1 | -1 (0.49190) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.77641 HOMO: -6.73210 LUMO: -2.49256 factor:1 | -1 (0.45389) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.51309 HOMO: -7.08040 LUMO: 0.84627 factor:1 | 1 (-1.28280) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.17815 HOMO: -7.00965 LUMO: 0.82995 factor:1 | 1 (-0.94785) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.98756 HOMO: -6.88448 LUMO: 0.82723 factor:1 | 1 (-0.75727) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.00277 HOMO: -7.20013 LUMO: 0.88437 factor:1 | 1 (-0.77248) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.40352 HOMO: -6.60420 LUMO: -0.53334 factor:1 | 1 (-0.17323) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.39182 HOMO: -6.78652 LUMO: -0.79729 factor:1 | 1 (-0.16153) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.11742 HOMO: -6.48992 LUMO: -0.64491 factor:1 | -1 (0.11287) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.33220 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-0.10191) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.17699 HOMO: -6.65046 LUMO: -0.78097 factor:1 | -1 (0.05331) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.49699 HOMO: -7.24095 LUMO: 0.37280 factor:1 | 1 (-0.26670) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.35612 HOMO: -6.81101 LUMO: -0.74831 factor:1 | 1 (-0.12583) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.59300 HOMO: -6.69400 LUMO: -0.77280 factor:1 | -1 (0.63729) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.17802 HOMO: -6.08447 LUMO: -0.68573 factor:1 | -1 (0.05227) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.91905 HOMO: -6.66679 LUMO: -0.47076 factor:1 | -1 (0.31124) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.36593 HOMO: -6.97428 LUMO: -1.10750 factor:1 | -1 (0.86437) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.30742 HOMO: -6.69128 LUMO: -0.54151 factor:1 | -1 (0.92287) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.10082 HOMO: -6.53617 LUMO: -0.35375 factor:1 | -1 (0.12947) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.93747 HOMO: -6.75659 LUMO: -0.41361 factor:1 | -1 (0.29282) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.97808 HOMO: -6.69400 LUMO: -0.67484 factor:1 | -1 (1.25221) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.75023 HOMO: -6.89264 LUMO: -0.90886 factor:1 | -1 (0.48006) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.01250 HOMO: -6.56339 LUMO: -0.52518 factor:1 | -1 (0.21780) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.10910 HOMO: -6.45726 LUMO: -0.65852 factor:1 | -1 (0.12120) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.27919 HOMO: -6.80557 LUMO: -0.56600 factor:1 | 1 (-0.04890) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.69888 HOMO: -7.19469 LUMO: -0.91702 factor:1 | -1 (0.53141) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.83674 HOMO: -6.41100 LUMO: 0.79185 factor:1 | -1 (0.39356) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.31357 HOMO: -6.39195 LUMO: 0.26123 factor:1 | -1 (0.91672) | -1 | -1 |
| G: -6154.86460 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.40484 HOMO: -6.78924 LUMO: 0.35919 factor:1 | -1 (0.82546) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.87518 HOMO: -6.50624 LUMO: 0.71838 factor:1 | -1 (0.92581) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.88217 HOMO: -6.68584 LUMO: -0.66124 factor:1 | -1 (0.91882) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.07427 HOMO: -6.45182 LUMO: -0.48980 factor:1 | 1 (-0.27328) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.87217 HOMO: -7.18925 LUMO: -1.01498 factor:1 | 1 (-1.07118) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.84066 HOMO: -7.18925 LUMO: -0.63130 factor:1 | 1 (-1.03967) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.85009 HOMO: -6.66679 LUMO: -0.57960 factor:1 | -1 (0.95090) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.31411 HOMO: -6.44910 LUMO: -0.30205 factor:1 | 1 (-0.51313) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.84819 HOMO: -7.23279 LUMO: 0.46804 factor:1 | 1 (-1.04720) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.80150 HOMO: -6.92802 LUMO: -0.72927 factor:1 | 1 (-1.00051) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.52938 HOMO: -6.83278 LUMO: -0.59321 factor:1 | 1 (-0.72839) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.65359 HOMO: -7.44776 LUMO: 0.27211 factor:1 | -1 (0.14740) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.54319 HOMO: -6.80829 LUMO: -0.59865 factor:1 | -1 (0.25780) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.51995 HOMO: -6.63686 LUMO: -0.75103 factor:1 | -1 (0.28104) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.32395 HOMO: -6.73210 LUMO: -0.55511 factor:1 | -1 (0.47704) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.59485 HOMO: -6.50624 LUMO: 1.58642 factor:1 | 1 (-0.79386) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.74863 HOMO: -6.79196 LUMO: 0.96328 factor:1 | -1 (0.05235) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.74751 HOMO: -6.82734 LUMO: 1.23540 factor:1 | 1 (-0.94652) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.90411 HOMO: -6.90081 LUMO: 1.25444 factor:1 | 1 (-1.10312) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.10181 HOMO: -7.00965 LUMO: -1.05036 factor:1 | 1 (-0.30082) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.26620 HOMO: -7.01237 LUMO: -1.48302 factor:1 | -1 (0.53479) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.16764 HOMO: -6.91713 LUMO: 0.93607 factor:1 | -1 (0.63335) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.77200 HOMO: -7.02598 LUMO: 0.92247 factor:1 | 1 (-0.97101) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.83295 HOMO: -6.98516 LUMO: 1.52384 factor:1 | 1 (-1.03196) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.38723 HOMO: -6.75387 LUMO: 1.04764 factor:1 | 1 (-0.58624) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.35103 HOMO: -7.09401 LUMO: 1.19458 factor:1 | -1 (1.44996) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.21513 HOMO: -6.88992 LUMO: -1.56193 factor:1 | -1 (0.58586) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.41683 HOMO: -7.00149 LUMO: 0.99866 factor:1 | -1 (1.38416) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.65989 HOMO: -7.13755 LUMO: 1.05308 factor:1 | 1 (-0.85890) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.99869 HOMO: -6.85183 LUMO: -1.42860 factor:1 | -1 (0.80230) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.50955 HOMO: -6.63141 LUMO: -0.88981 factor:1 | 1 (-0.70856) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.55601 HOMO: -6.92258 LUMO: -0.82178 factor:1 | -1 (0.24498) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.08329 HOMO: -6.55794 LUMO: -0.80818 factor:1 | -1 (0.71770) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.07118 HOMO: -6.95251 LUMO: -0.97145 factor:1 | -1 (0.72981) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.70677 HOMO: -7.37701 LUMO: 0.14150 factor:1 | -1 (1.09422) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.60643 HOMO: -6.74842 LUMO: -0.68028 factor:1 | -1 (0.19456) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.75052 HOMO: -6.65046 LUMO: -0.52518 factor:1 | -1 (1.05047) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12414.84417 HOMO: -6.91441 LUMO: -1.13199 factor:1 | -1 (2.95682) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.77580 HOMO: -7.00965 LUMO: -1.00682 factor:1 | -1 (1.02519) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.30284 HOMO: -6.55794 LUMO: -0.54967 factor:1 | -1 (1.49815) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.56772 HOMO: -6.71577 LUMO: -0.53879 factor:1 | -1 (1.23327) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.45343 HOMO: -6.88992 LUMO: -0.55511 factor:1 | -1 (1.34756) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12414.78776 HOMO: -6.74026 LUMO: -0.60681 factor:1 | -1 (3.01323) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.69659 HOMO: -6.76747 LUMO: -0.50885 factor:1 | -1 (1.10440) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.77841 HOMO: -6.87904 LUMO: -0.92519 factor:1 | -1 (1.02258) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.72726 HOMO: -6.53073 LUMO: -0.53062 factor:1 | -1 (1.07373) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12414.96322 HOMO: -6.97700 LUMO: -0.98505 factor:1 | -1 (2.83777) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.10646 HOMO: -6.96884 LUMO: -0.79185 factor:1 | -1 (1.69453) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.49272 HOMO: -6.60420 LUMO: -0.31021 factor:1 | -1 (1.30827) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.59144 HOMO: -6.68584 LUMO: -0.63947 factor:1 | -1 (1.20955) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12414.36297 HOMO: -6.41917 LUMO: -0.35103 factor:1 | -1 (3.43802) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.21822 HOMO: -6.73482 LUMO: -0.70477 factor:1 | 1 (-0.41723) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.35857 HOMO: -6.71305 LUMO: -0.85716 factor:1 | 1 (-1.55758) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.42163 HOMO: -6.70761 LUMO: -0.63403 factor:1 | 1 (-0.62064) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.33519 HOMO: -6.37563 LUMO: -0.38640 factor:1 | 1 (-1.53421) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.48576 HOMO: -6.27495 LUMO: -0.54967 factor:1 | 1 (-0.68477) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.23750 HOMO: -6.98516 LUMO: 0.38096 factor:1 | 1 (-2.43651) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.63931 HOMO: -6.47087 LUMO: -0.40001 factor:1 | 1 (-1.83832) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.66741 HOMO: -6.59876 LUMO: 0.20681 factor:1 | 1 (-2.86642) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.91248 HOMO: -6.89809 LUMO: 0.14966 factor:1 | 1 (-3.11149) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.76267 HOMO: -6.76203 LUMO: 2.11432 factor:1 | 1 (-0.96168) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.83619 HOMO: -6.58516 LUMO: 1.75786 factor:1 | 1 (-1.03520) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.16359 HOMO: -6.37835 LUMO: 1.84493 factor:1 | 1 (-2.36260) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.44961 HOMO: -6.83550 LUMO: 1.74425 factor:1 | 1 (-2.64862) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.83490 HOMO: -6.65318 LUMO: 1.79051 factor:1 | 1 (-2.03392) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.32219 HOMO: -6.68584 LUMO: 2.11160 factor:1 | 1 (-1.52120) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.97054 HOMO: -6.36202 LUMO: 1.85037 factor:1 | 1 (-1.16955) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.65096 HOMO: -6.68312 LUMO: 2.23133 factor:1 | 1 (-1.84997) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.40088 HOMO: -6.66679 LUMO: 2.14154 factor:1 | 1 (-1.59989) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.04528 HOMO: -6.50896 LUMO: 1.92657 factor:1 | 1 (-1.24430) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.87690 HOMO: -6.63686 LUMO: 2.22317 factor:1 | 1 (-1.07591) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.36951 HOMO: -6.58788 LUMO: 2.17419 factor:1 | 1 (-1.56852) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.73975 HOMO: -6.72665 LUMO: 2.12249 factor:1 | 1 (-1.93876) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.43677 HOMO: -6.28311 LUMO: 1.91024 factor:1 | 1 (-1.63579) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.16125 HOMO: -6.56067 LUMO: 2.27487 factor:1 | 1 (-2.36026) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.20208 HOMO: -6.83006 LUMO: 2.28031 factor:1 | 1 (-1.40109) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.34191 HOMO: -6.45182 LUMO: 1.62724 factor:1 | -1 (0.45908) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.32809 HOMO: -6.78380 LUMO: 1.83677 factor:1 | 1 (-1.52710) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.89828 HOMO: -6.23413 LUMO: 1.80956 factor:1 | 1 (-2.09729) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.40110 HOMO: -6.74298 LUMO: 2.16875 factor:1 | 1 (-1.60011) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.31650 HOMO: -6.81645 LUMO: 2.50073 factor:1 | 1 (-1.51551) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.32894 HOMO: -6.71033 LUMO: 1.96466 factor:1 | 1 (-1.52795) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.59589 HOMO: -6.83550 LUMO: 2.04358 factor:1 | 1 (-0.79490) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.30815 HOMO: -6.60965 LUMO: 2.38100 factor:1 | 1 (-1.50716) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.09236 HOMO: -6.73210 LUMO: 2.26127 factor:1 | 1 (-1.29137) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.44302 HOMO: -6.76203 LUMO: 2.13609 factor:1 | 1 (-0.64203) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.31627 HOMO: -6.71033 LUMO: 2.05990 factor:1 | 1 (-2.51528) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.31630 HOMO: -6.50896 LUMO: 2.32385 factor:1 | 1 (-2.51531) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.10022 HOMO: -6.53345 LUMO: 1.74425 factor:1 | 1 (-2.29923) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.54515 HOMO: -6.25862 LUMO: 1.63540 factor:1 | 1 (-2.74416) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.93077 HOMO: -5.90759 LUMO: 1.78779 factor:1 | 1 (-2.12978) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.86347 HOMO: -6.09807 LUMO: 1.99732 factor:1 | 1 (-3.06248) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.29546 HOMO: -5.92392 LUMO: 1.99732 factor:1 | 1 (-2.49447) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.87560 HOMO: -6.45182 LUMO: 1.72248 factor:1 | 1 (-3.07461) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.47921 HOMO: -6.53073 LUMO: 1.82588 factor:1 | 1 (-0.67822) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.17737 HOMO: -6.40828 LUMO: 2.05174 factor:1 | 1 (-1.37638) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.98327 HOMO: -6.60420 LUMO: -0.82450 factor:1 | 1 (-1.18228) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.55344 HOMO: -6.76747 LUMO: -0.57144 factor:1 | 1 (-0.75245) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.73384 HOMO: -6.67767 LUMO: -0.59321 factor:1 | 1 (-1.93285) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.74705 HOMO: -6.65863 LUMO: -0.57416 factor:1 | 1 (-0.94606) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.54025 HOMO: -6.49808 LUMO: -0.54695 factor:1 | 1 (-2.73926) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.84982 HOMO: -6.50080 LUMO: -0.61498 factor:1 | 1 (-2.04883) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.58107 HOMO: -6.74842 LUMO: -0.51974 factor:1 | 1 (-2.78008) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.71248 HOMO: -6.13345 LUMO: 0.67756 factor:1 | 1 (-1.91149) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.17235 HOMO: -6.48719 LUMO: 0.52790 factor:1 | 1 (-2.37136) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.72208 HOMO: -6.35930 LUMO: 0.74015 factor:1 | -1 (0.07891) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.95228 HOMO: -6.41644 LUMO: 0.22313 factor:1 | 1 (-1.15129) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.01535 HOMO: -6.85727 LUMO: -0.00272 factor:1 | 1 (-1.21436) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.94387 HOMO: -6.84638 LUMO: 0.24762 factor:1 | 1 (-1.14288) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.05453 HOMO: -6.66951 LUMO: 0.39184 factor:1 | 1 (-2.25354) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.84503 HOMO: -6.62597 LUMO: -0.65035 factor:1 | 1 (-2.04404) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.69392 HOMO: -7.13755 LUMO: 0.45715 factor:1 | 1 (-1.89293) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.07129 HOMO: -7.12666 LUMO: 0.45171 factor:1 | 1 (-2.27030) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.40061 HOMO: -6.46270 LUMO: -0.46259 factor:1 | 1 (-1.59962) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.62921 HOMO: -6.36202 LUMO: -0.29660 factor:1 | 1 (-1.82822) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.18253 HOMO: -6.28583 LUMO: 0.40545 factor:1 | 1 (-2.38154) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.45726 HOMO: -6.70761 LUMO: 0.41906 factor:1 | 1 (-2.65627) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.82671 HOMO: -6.76203 LUMO: -0.60954 factor:1 | 1 (-3.02572) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.34076 HOMO: -6.85999 LUMO: -0.75103 factor:1 | 1 (-2.53977) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.77969 HOMO: -7.19741 LUMO: -1.00954 factor:1 | 1 (-1.97870) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.06797 HOMO: -6.58243 LUMO: -0.33470 factor:1 | 1 (-2.26698) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.07151 HOMO: -7.22190 LUMO: 0.49253 factor:1 | 1 (-2.27052) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.14958 HOMO: -7.22462 LUMO: 0.51974 factor:1 | 1 (-2.34859) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.56572 HOMO: -7.08584 LUMO: -0.68301 factor:1 | 1 (-2.76473) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.46958 HOMO: -6.68584 LUMO: -0.29660 factor:1 | 1 (-2.66859) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.99972 HOMO: -6.33753 LUMO: -0.48436 factor:1 | 1 (-2.19873) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.29238 HOMO: -7.15932 LUMO: 0.55511 factor:1 | 1 (-2.49139) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.18776 HOMO: -6.57427 LUMO: 2.01908 factor:1 | 1 (-1.38677) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.79586 HOMO: -6.75659 LUMO: 2.22045 factor:1 | 1 (-1.99487) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.69151 HOMO: -6.73482 LUMO: 2.20956 factor:1 | 1 (-0.89052) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.74770 HOMO: -6.74026 LUMO: 1.76602 factor:1 | 1 (-0.94671) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.86564 HOMO: -6.95523 LUMO: 1.94834 factor:1 | 1 (-3.06466) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.38257 HOMO: -6.33209 LUMO: 1.87486 factor:1 | 1 (-1.58158) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.40821 HOMO: -6.71033 LUMO: 2.12521 factor:1 | 1 (-0.60722) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.13865 HOMO: -6.50080 LUMO: 2.04902 factor:1 | 1 (-1.33766) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.03720 HOMO: -6.76475 LUMO: 1.94017 factor:1 | 1 (-1.23621) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.23460 HOMO: -6.53073 LUMO: 2.08983 factor:1 | 1 (-0.43361) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.39191 HOMO: -6.69944 LUMO: 2.20684 factor:1 | 1 (-0.59092) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.83671 HOMO: -6.34570 LUMO: 1.80684 factor:1 | 1 (-1.03572) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.15497 HOMO: -6.78380 LUMO: 1.95922 factor:1 | 1 (-1.35398) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.80302 HOMO: -6.93618 LUMO: 1.76058 factor:1 | 1 (-1.00203) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.15910 HOMO: -6.93346 LUMO: 1.79595 factor:1 | 1 (-2.35811) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.49144 HOMO: -6.29671 LUMO: 1.75241 factor:1 | 1 (-1.69045) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.27682 HOMO: -6.77019 LUMO: 1.74697 factor:1 | 1 (-2.47583) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.78677 HOMO: -6.87360 LUMO: 1.91024 factor:1 | 1 (-1.98578) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.25154 HOMO: -6.32665 LUMO: 1.87759 factor:1 | 1 (-2.45055) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12421.04709 HOMO: -6.99877 LUMO: 1.99187 factor:1 | 1 (-3.24610) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.07515 HOMO: -6.72665 LUMO: 2.12521 factor:1 | 1 (-2.27416) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.60791 HOMO: -6.67767 LUMO: 2.43814 factor:1 | 1 (-1.80692) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.55827 HOMO: -6.99605 LUMO: 1.79051 factor:1 | 1 (-1.75728) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.54790 HOMO: -6.25046 LUMO: 1.77146 factor:1 | 1 (-2.74691) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.25363 HOMO: -6.30488 LUMO: 1.90480 factor:1 | 1 (-2.45264) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.10533 HOMO: -6.38379 LUMO: 1.68438 factor:1 | 1 (-2.30434) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.13344 HOMO: -6.78924 LUMO: 2.01364 factor:1 | 1 (-2.33245) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.78127 HOMO: -6.15249 LUMO: 1.98643 factor:1 | 1 (-1.98028) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.91485 HOMO: -6.19331 LUMO: 2.14154 factor:1 | 1 (-2.11386) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.05337 HOMO: -6.05998 LUMO: 2.12521 factor:1 | 1 (-1.25238) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.58105 HOMO: -6.67223 LUMO: 1.91840 factor:1 | 1 (-1.78006) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.18431 HOMO: -6.79196 LUMO: 2.18507 factor:1 | 1 (-1.38332) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.44478 HOMO: -6.93346 LUMO: 1.78235 factor:1 | 1 (-1.64379) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.07043 HOMO: -6.16882 LUMO: 1.80956 factor:1 | 1 (-1.26944) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.85608 HOMO: -6.72665 LUMO: 2.07895 factor:1 | 1 (-1.05509) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.06997 HOMO: -6.73210 LUMO: 1.97827 factor:1 | 1 (-1.26898) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.79886 HOMO: -6.84638 LUMO: 1.87214 factor:1 | 1 (-0.99787) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.53733 HOMO: -6.83006 LUMO: 2.36195 factor:1 | 1 (-0.73634) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.60179 HOMO: -6.97700 LUMO: 1.91024 factor:1 | 1 (-0.80080) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.77829 HOMO: -6.20420 LUMO: 1.81772 factor:1 | 1 (-0.97730) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.98814 HOMO: -7.09129 LUMO: 2.10344 factor:1 | 1 (-1.18715) | 1 | 1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.30297 HOMO: -6.77564 LUMO: 2.14970 factor:1 | 1 (-2.50198) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.99387 HOMO: -6.81645 LUMO: 1.85854 factor:1 | 1 (-2.19288) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.64995 HOMO: -6.50896 LUMO: 2.04358 factor:1 | 1 (-1.84896) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.39494 HOMO: -6.89264 LUMO: 1.66262 factor:1 | 1 (-2.59395) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.39361 HOMO: -6.75931 LUMO: 2.23950 factor:1 | 1 (-2.59262) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.95427 HOMO: -6.50080 LUMO: 1.67622 factor:1 | 1 (-3.15328) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.29886 HOMO: -6.30216 LUMO: 2.24222 factor:1 | 1 (-2.49787) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.30302 HOMO: -7.18108 LUMO: 2.10072 factor:1 | 1 (-2.50203) | 1 | 1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.97895 HOMO: -6.54162 LUMO: 2.35378 factor:1 | 1 (-3.17796) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.63451 HOMO: -5.98650 LUMO: 1.48302 factor:1 | 1 (-2.83352) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.30942 HOMO: -7.15115 LUMO: 2.14970 factor:1 | 1 (-2.50843) | 1 | 1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.61288 HOMO: -6.45454 LUMO: 2.15786 factor:1 | 1 (-2.81189) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.01107 HOMO: -7.06952 LUMO: 2.14970 factor:1 | 1 (-2.21008) | 1 | 1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.28224 HOMO: -6.93618 LUMO: 1.86942 factor:1 | 1 (-1.48125) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.27786 HOMO: -6.63141 LUMO: 1.92657 factor:1 | 1 (-1.47687) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.96795 HOMO: -6.51441 LUMO: -0.44355 factor:1 | 1 (-1.16696) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.83304 HOMO: -6.82734 LUMO: -1.03131 factor:1 | 1 (-1.03205) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.98569 HOMO: -6.58788 LUMO: -0.82995 factor:1 | 1 (-1.18470) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.82947 HOMO: -6.43277 LUMO: -0.40817 factor:1 | 1 (-1.02848) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.78305 HOMO: -6.78924 LUMO: -0.72110 factor:1 | 1 (-0.98206) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.79540 HOMO: -7.28177 LUMO: 0.36735 factor:1 | 1 (-0.99441) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.67292 HOMO: -6.47903 LUMO: -0.46259 factor:1 | 1 (-0.87193) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.63710 HOMO: -6.67495 LUMO: -0.75376 factor:1 | 1 (-2.83611) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.84701 HOMO: -6.71033 LUMO: -0.71838 factor:1 | 1 (-2.04602) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.10375 HOMO: -6.79740 LUMO: -0.79185 factor:1 | 1 (-2.30276) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.25720 HOMO: -6.08719 LUMO: -0.63675 factor:1 | 1 (-2.45621) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.39218 HOMO: -6.84094 LUMO: 0.42994 factor:1 | 1 (-1.59119) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.14016 HOMO: -6.59604 LUMO: 0.25851 factor:1 | 1 (-2.33917) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.69169 HOMO: -6.82462 LUMO: 0.08708 factor:1 | 1 (-1.89070) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.44305 HOMO: -6.54706 LUMO: 0.44082 factor:1 | 1 (-2.64206) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.99513 HOMO: -6.99333 LUMO: 0.32109 factor:1 | 1 (-1.19414) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.18088 HOMO: -6.29944 LUMO: -0.57144 factor:1 | 1 (-1.37989) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.51562 HOMO: -6.57699 LUMO: -0.46531 factor:1 | 1 (-2.71464) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.71351 HOMO: -6.24773 LUMO: -0.53879 factor:1 | 1 (-1.91253) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.57449 HOMO: -6.96067 LUMO: -0.67212 factor:1 | 1 (-1.77350) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.94361 HOMO: -7.24095 LUMO: -0.09252 factor:1 | 1 (-2.14262) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.44835 HOMO: -6.33481 LUMO: -0.46531 factor:1 | 1 (-0.64736) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.46999 HOMO: -6.43549 LUMO: -0.33198 factor:1 | -1 (0.33100) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.36678 HOMO: -6.53073 LUMO: 0.44899 factor:1 | 1 (-2.56579) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.54997 HOMO: -6.69128 LUMO: 0.47620 factor:1 | 1 (-1.74898) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.47264 HOMO: -6.65318 LUMO: 0.52246 factor:1 | 1 (-1.67165) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.55436 HOMO: -6.71305 LUMO: 0.41089 factor:1 | 1 (-0.75337) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.04998 HOMO: -6.70216 LUMO: 0.19864 factor:1 | 1 (-2.24899) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.16052 HOMO: -6.41100 LUMO: 0.34558 factor:1 | 1 (-1.35954) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.12726 HOMO: -7.01237 LUMO: 0.02993 factor:1 | 1 (-2.32627) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.11978 HOMO: -6.85999 LUMO: 0.18776 factor:1 | -1 (0.68121) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.12572 HOMO: -6.62869 LUMO: 0.48708 factor:1 | 1 (-1.32473) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.41513 HOMO: -6.43821 LUMO: -0.45715 factor:1 | -1 (0.38586) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.28872 HOMO: -6.43277 LUMO: -0.72110 factor:1 | 1 (-1.48773) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.22945 HOMO: -7.10761 LUMO: 0.43266 factor:1 | 1 (-1.42846) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.98977 HOMO: -6.57699 LUMO: -0.61498 factor:1 | 1 (-1.18878) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.24398 HOMO: -6.82189 LUMO: -0.75648 factor:1 | 1 (-1.44299) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.82879 HOMO: -6.55794 LUMO: -0.67212 factor:1 | 1 (-1.02780) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.88681 HOMO: -6.69128 LUMO: 1.88575 factor:1 | 1 (-1.08582) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.79616 HOMO: -6.65591 LUMO: 1.70888 factor:1 | 1 (-0.99517) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.76634 HOMO: -6.58788 LUMO: 1.68438 factor:1 | 1 (-0.96535) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.35993 HOMO: -6.46270 LUMO: 1.72520 factor:1 | 1 (-1.55894) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.07467 HOMO: -6.57427 LUMO: 1.73881 factor:1 | 1 (-1.27368) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.18072 HOMO: -6.45182 LUMO: 1.75241 factor:1 | 1 (-1.37973) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.72514 HOMO: -6.51441 LUMO: 1.78779 factor:1 | 1 (-0.92415) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.44061 HOMO: -6.67495 LUMO: 2.11705 factor:1 | 1 (-1.63962) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.59989 HOMO: -6.22597 LUMO: 1.96466 factor:1 | 1 (-0.79890) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.35830 HOMO: -6.68040 LUMO: 2.30753 factor:1 | 1 (-1.55731) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.09492 HOMO: -6.65046 LUMO: 2.18235 factor:1 | 1 (-1.29393) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.28183 HOMO: -6.38651 LUMO: 1.76874 factor:1 | 1 (-1.48084) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.36037 HOMO: -6.41644 LUMO: 2.09256 factor:1 | 1 (-1.55938) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.95590 HOMO: -6.14977 LUMO: 2.28031 factor:1 | 1 (-1.15491) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.25574 HOMO: -6.70489 LUMO: 2.43814 factor:1 | 1 (-1.45475) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.66800 HOMO: -6.78924 LUMO: 2.27215 factor:1 | 1 (-0.86701) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.89349 HOMO: -6.86271 LUMO: 2.31025 factor:1 | 1 (-2.09250) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.19107 HOMO: -6.51168 LUMO: 2.04630 factor:1 | 1 (-2.39008) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.33356 HOMO: -6.72665 LUMO: 2.13337 factor:1 | 1 (-1.53257) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.96479 HOMO: -6.45998 LUMO: 2.16058 factor:1 | 1 (-1.16380) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.92348 HOMO: -6.83822 LUMO: 2.20684 factor:1 | 1 (-2.12249) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.03424 HOMO: -6.68856 LUMO: 2.19324 factor:1 | 1 (-1.23325) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.98711 HOMO: -6.71577 LUMO: 2.16058 factor:1 | 1 (-1.18612) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.05652 HOMO: -6.82462 LUMO: 1.90208 factor:1 | 1 (-1.25553) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.25555 HOMO: -6.61509 LUMO: 2.23950 factor:1 | 1 (-1.45456) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.35601 HOMO: -6.73754 LUMO: 1.84221 factor:1 | 1 (-1.55502) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.42031 HOMO: -6.56611 LUMO: 1.94561 factor:1 | 1 (-1.61932) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.91919 HOMO: -6.67767 LUMO: 1.51840 factor:1 | 1 (-1.11820) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.75128 HOMO: -6.35658 LUMO: 2.16603 factor:1 | 1 (-1.95029) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.49695 HOMO: -6.35114 LUMO: 2.08983 factor:1 | 1 (-0.69596) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.26763 HOMO: -6.35114 LUMO: 2.10616 factor:1 | 1 (-1.46664) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.09364 HOMO: -6.71305 LUMO: 2.01636 factor:1 | 1 (-1.29265) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.35743 HOMO: -6.24773 LUMO: 1.98915 factor:1 | 1 (-1.55644) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.42420 HOMO: -6.53617 LUMO: 2.42726 factor:1 | 1 (-1.62321) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.34847 HOMO: -6.59332 LUMO: 1.82316 factor:1 | 1 (-2.54748) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.59556 HOMO: -6.41372 LUMO: 1.77418 factor:1 | 1 (-0.79457) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.04903 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-2.24804) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.77520 HOMO: -6.11168 LUMO: 1.70888 factor:1 | 1 (-1.97421) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.25053 HOMO: -6.44910 LUMO: 2.23405 factor:1 | 1 (-2.44954) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.50720 HOMO: -6.24773 LUMO: 2.12793 factor:1 | 1 (-1.70621) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.16367 HOMO: -6.07358 LUMO: 1.89663 factor:1 | 1 (-2.36268) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.10555 HOMO: -6.66679 LUMO: 1.96738 factor:1 | 1 (-2.30456) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.38967 HOMO: -6.68312 LUMO: 1.78235 factor:1 | 1 (-1.58868) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.82103 HOMO: -6.70761 LUMO: 1.97555 factor:1 | 1 (-2.02004) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.46937 HOMO: -6.15794 LUMO: 2.00548 factor:1 | 1 (-1.66838) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.80780 HOMO: -6.52257 LUMO: 1.96738 factor:1 | 1 (-2.00681) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.18088 HOMO: -6.25590 LUMO: 1.86670 factor:1 | 1 (-1.37989) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.97074 HOMO: -6.30216 LUMO: 1.84765 factor:1 | 1 (-2.16975) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.82144 HOMO: -6.76747 LUMO: 2.20956 factor:1 | 1 (-2.02045) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.04654 HOMO: -6.14161 LUMO: 1.80684 factor:1 | 1 (-1.24555) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.64853 HOMO: -6.81373 LUMO: 1.91024 factor:1 | 1 (-1.84754) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.72208 HOMO: -6.81917 LUMO: 2.34834 factor:1 | -1 (0.07891) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.43487 HOMO: -6.72121 LUMO: 1.90208 factor:1 | 1 (-1.63388) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.36078 HOMO: -7.51851 LUMO: 0.26939 factor:1 | 1 (-0.55979) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.80487 HOMO: -6.65318 LUMO: -0.57144 factor:1 | 1 (-1.00388) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.34793 HOMO: -6.77564 LUMO: -0.72654 factor:1 | 1 (-1.54694) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.42662 HOMO: -6.80557 LUMO: -0.60954 factor:1 | 1 (-2.62563) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.25010 HOMO: -7.35524 LUMO: 0.27483 factor:1 | 1 (-1.44912) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.99819 HOMO: -6.94979 LUMO: -0.83811 factor:1 | 1 (-3.19720) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.58861 HOMO: -6.13345 LUMO: -0.67212 factor:1 | 1 (-1.78762) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.54445 HOMO: -6.47359 LUMO: -0.59321 factor:1 | 1 (-1.74346) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.79126 HOMO: -6.52257 LUMO: -0.54695 factor:1 | 1 (-1.99027) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.37785 HOMO: -6.61781 LUMO: -0.69661 factor:1 | 1 (-2.57686) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.85732 HOMO: -6.77564 LUMO: -0.80001 factor:1 | 1 (-3.05633) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.89041 HOMO: -7.35252 LUMO: -1.00410 factor:1 | 1 (-3.08942) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.77335 HOMO: -6.35386 LUMO: -0.38912 factor:1 | 1 (-1.97236) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.03654 HOMO: -6.80285 LUMO: -0.52246 factor:1 | 1 (-2.23555) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.76640 HOMO: -7.23279 LUMO: 0.30477 factor:1 | 1 (-0.96541) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.55344 HOMO: -7.13483 LUMO: -0.76192 factor:1 | 1 (-0.75245) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.49893 HOMO: -6.71849 LUMO: -0.48164 factor:1 | 1 (-1.69794) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.92511 HOMO: -6.85455 LUMO: -0.69389 factor:1 | 1 (-2.12412) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.55369 HOMO: -6.96339 LUMO: -0.73743 factor:1 | 1 (-2.75270) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.71025 HOMO: -7.50490 LUMO: 0.28844 factor:1 | 1 (-1.90926) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.83292 HOMO: -6.63958 LUMO: -0.50069 factor:1 | 1 (-2.03193) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.95641 HOMO: -6.78924 LUMO: -0.69661 factor:1 | 1 (-1.15542) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.32532 HOMO: -7.44776 LUMO: 0.33742 factor:1 | 1 (-1.52433) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.75290 HOMO: -6.15249 LUMO: 0.66396 factor:1 | 1 (-0.95191) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.86403 HOMO: -6.17426 LUMO: 0.55511 factor:1 | 1 (-1.06304) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.08675 HOMO: -6.83550 LUMO: 0.28844 factor:1 | 1 (-1.28577) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.91029 HOMO: -6.32393 LUMO: 0.47620 factor:1 | 1 (-1.10930) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.73869 HOMO: -6.32937 LUMO: 0.45987 factor:1 | 1 (-0.93770) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.89257 HOMO: -7.37429 LUMO: 0.09252 factor:1 | 1 (-2.09158) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.32784 HOMO: -6.54434 LUMO: -0.39729 factor:1 | 1 (-2.52685) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.81137 HOMO: -7.35524 LUMO: 0.28028 factor:1 | 1 (-2.01038) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.33867 HOMO: -6.95523 LUMO: -0.86804 factor:1 | 1 (-2.53768) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.93684 HOMO: -6.63958 LUMO: -0.65307 factor:1 | 1 (-2.13585) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.85096 HOMO: -6.73482 LUMO: -0.67212 factor:1 | 1 (-2.04997) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.33086 HOMO: -6.37835 LUMO: -0.53606 factor:1 | 1 (-2.52987) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.71783 HOMO: -6.71849 LUMO: -0.61226 factor:1 | 1 (-2.91684) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.85942 HOMO: -6.68584 LUMO: -1.11022 factor:1 | 1 (-2.05843) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.76026 HOMO: -6.80285 LUMO: -0.79185 factor:1 | 1 (-2.95927) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.75708 HOMO: -7.14571 LUMO: -0.94696 factor:1 | 1 (-1.95609) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.21995 HOMO: -7.16204 LUMO: -0.66124 factor:1 | 1 (-2.41896) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.23091 HOMO: -6.54978 LUMO: -0.54967 factor:1 | 1 (-2.42992) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.12071 HOMO: -6.75114 LUMO: -0.70750 factor:1 | 1 (-2.31972) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.06610 HOMO: -7.22190 LUMO: 0.39184 factor:1 | 1 (-1.26511) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.02177 HOMO: -7.43959 LUMO: 0.30477 factor:1 | 1 (-1.22078) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.25293 HOMO: -6.87360 LUMO: -0.77552 factor:1 | 1 (-2.45194) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.62795 HOMO: -6.82734 LUMO: -0.59593 factor:1 | 1 (-2.82696) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.92230 HOMO: -6.65318 LUMO: -0.46259 factor:1 | 1 (-3.12131) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.25056 HOMO: -7.05863 LUMO: -1.17009 factor:1 | 1 (-2.44957) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.81732 HOMO: -6.57427 LUMO: -0.48708 factor:1 | 1 (-3.01633) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.77250 HOMO: -6.60420 LUMO: -0.38096 factor:1 | 1 (-2.97151) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.99099 HOMO: -6.72121 LUMO: -0.66668 factor:1 | 1 (-2.19000) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.49271 HOMO: -6.52257 LUMO: -0.19320 factor:1 | 1 (-2.69172) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.07720 HOMO: -6.28039 LUMO: -0.27211 factor:1 | 1 (-1.27621) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.09756 HOMO: -6.71849 LUMO: -0.42722 factor:1 | 1 (-1.29657) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.00743 HOMO: -6.27495 LUMO: 0.27756 factor:1 | 1 (-1.20644) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.61344 HOMO: -6.21780 LUMO: 0.46531 factor:1 | 1 (-0.81245) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.64305 HOMO: -6.52257 LUMO: -0.64491 factor:1 | 1 (-0.84206) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.45182 HOMO: -6.73754 LUMO: 1.83133 factor:1 | 1 (-1.65083) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.45045 HOMO: -6.67223 LUMO: 1.88847 factor:1 | 1 (-2.64946) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.60037 HOMO: -6.82189 LUMO: 1.59187 factor:1 | 1 (-1.79938) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.45634 HOMO: -6.43277 LUMO: 1.76330 factor:1 | 1 (-1.65535) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.02215 HOMO: -6.48175 LUMO: 1.77962 factor:1 | 1 (-2.22116) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.93355 HOMO: -6.50352 LUMO: 1.68438 factor:1 | 1 (-1.13257) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.28956 HOMO: -6.31576 LUMO: 2.03813 factor:1 | 1 (-1.48857) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.62529 HOMO: -6.27495 LUMO: 1.99459 factor:1 | 1 (-2.82430) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.91661 HOMO: -6.23957 LUMO: 2.17147 factor:1 | 1 (-3.11562) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12421.01582 HOMO: -6.78108 LUMO: 2.16875 factor:1 | 1 (-3.21483) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.08696 HOMO: -6.34297 LUMO: 2.10344 factor:1 | 1 (-2.28597) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.66909 HOMO: -6.30216 LUMO: 2.00004 factor:1 | 1 (-0.86810) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.64291 HOMO: -6.72665 LUMO: 2.09528 factor:1 | 1 (-0.84192) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.61140 HOMO: -6.86543 LUMO: 1.91568 factor:1 | 1 (-0.81041) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.58473 HOMO: -5.83956 LUMO: 1.89391 factor:1 | 1 (-0.78374) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.74925 HOMO: -6.42189 LUMO: 2.03269 factor:1 | 1 (-0.94826) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.69509 HOMO: -6.07630 LUMO: 1.80956 factor:1 | 1 (-1.89410) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.56617 HOMO: -6.43277 LUMO: 1.81772 factor:1 | 1 (-0.76518) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.15503 HOMO: -7.03959 LUMO: 1.78779 factor:1 | 1 (-1.35404) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.30668 HOMO: -6.72121 LUMO: 2.29664 factor:1 | 1 (-1.50569) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.31471 HOMO: -6.62869 LUMO: 2.04630 factor:1 | 1 (-0.51372) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.14679 HOMO: -6.63958 LUMO: 1.84221 factor:1 | 1 (-0.34580) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.99327 HOMO: -6.70761 LUMO: 1.67350 factor:1 | 1 (-0.19228) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.40322 HOMO: -6.00283 LUMO: 1.64357 factor:1 | 1 (-1.60223) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.25295 HOMO: -6.48719 LUMO: 1.70343 factor:1 | 1 (-2.45196) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.12569 HOMO: -6.13345 LUMO: 1.44492 factor:1 | 1 (-2.32470) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.98010 HOMO: -6.11168 LUMO: 1.70071 factor:1 | 1 (-2.17912) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.54766 HOMO: -6.09535 LUMO: 1.82316 factor:1 | 1 (-1.74667) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.34483 HOMO: -6.81101 LUMO: 1.63540 factor:1 | 1 (-1.54384) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.52034 HOMO: -6.80013 LUMO: 2.12249 factor:1 | 1 (-1.71935) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.74116 HOMO: -6.48447 LUMO: 1.94561 factor:1 | 1 (-1.94017) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.53315 HOMO: -6.72393 LUMO: 2.06534 factor:1 | 1 (-2.73216) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.11791 HOMO: -6.34570 LUMO: 1.98915 factor:1 | 1 (-1.31692) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.53259 HOMO: -6.31304 LUMO: 1.87759 factor:1 | 1 (-1.73160) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.72383 HOMO: -6.77564 LUMO: 1.81228 factor:1 | 1 (-1.92284) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.02079 HOMO: -6.58516 LUMO: 2.34834 factor:1 | 1 (-2.21980) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.53457 HOMO: -6.68040 LUMO: 2.20412 factor:1 | 1 (-1.73358) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.72415 HOMO: -6.20964 LUMO: 2.17147 factor:1 | 1 (-1.92316) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.88576 HOMO: -6.54706 LUMO: 2.03813 factor:1 | 1 (-2.08477) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.22351 HOMO: -6.54162 LUMO: 2.17419 factor:1 | 1 (-2.42252) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.95425 HOMO: -6.75659 LUMO: 2.22589 factor:1 | 1 (-2.15326) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.31158 HOMO: -6.59604 LUMO: 2.59325 factor:1 | 1 (-1.51059) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.46703 HOMO: -6.11712 LUMO: 2.02181 factor:1 | 1 (-1.66604) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.60924 HOMO: -6.63141 LUMO: 2.09256 factor:1 | 1 (-1.80825) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.65613 HOMO: -6.61781 LUMO: 1.86126 factor:1 | 1 (-0.85515) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.60634 HOMO: -6.63958 LUMO: 1.77146 factor:1 | 1 (-0.80535) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.71619 HOMO: -6.60420 LUMO: 1.54561 factor:1 | 1 (-0.91520) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.34926 HOMO: -6.52529 LUMO: 2.05174 factor:1 | 1 (-1.54827) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.41553 HOMO: -6.80285 LUMO: 2.13609 factor:1 | 1 (-0.61454) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.24826 HOMO: -6.51168 LUMO: 2.25855 factor:1 | 1 (-0.44727) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.49115 HOMO: -6.64774 LUMO: 2.46263 factor:1 | 1 (-0.69016) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.65173 HOMO: -6.40828 LUMO: 1.99732 factor:1 | 1 (-0.85074) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.90787 HOMO: -5.97562 LUMO: 1.56465 factor:1 | 1 (-1.10688) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.81431 HOMO: -6.75659 LUMO: 2.23405 factor:1 | 1 (-1.01332) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.43955 HOMO: -6.68584 LUMO: 2.09528 factor:1 | 1 (-1.63856) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.97309 HOMO: -6.86543 LUMO: 1.95106 factor:1 | 1 (-1.17210) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.76933 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-0.96834) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.45281 HOMO: -6.87632 LUMO: 2.08439 factor:1 | 1 (-0.65182) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.54781 HOMO: -6.33753 LUMO: 2.16603 factor:1 | 1 (-0.74682) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.41180 HOMO: -6.92258 LUMO: 1.72248 factor:1 | 1 (-0.61081) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.63627 HOMO: -6.62597 LUMO: 2.10344 factor:1 | 1 (-0.83528) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.59573 HOMO: -6.63141 LUMO: 1.94017 factor:1 | 1 (-0.79474) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.73935 HOMO: -6.48447 LUMO: 1.91840 factor:1 | 1 (-0.93836) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.16050 HOMO: -6.41372 LUMO: 1.61364 factor:1 | 1 (-1.35951) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.59520 HOMO: -6.37291 LUMO: 1.79051 factor:1 | 1 (-1.79421) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.06536 HOMO: -6.13073 LUMO: 1.77962 factor:1 | 1 (-2.26437) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.45601 HOMO: -6.13073 LUMO: 1.98915 factor:1 | 1 (-1.65502) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.46673 HOMO: -6.44094 LUMO: 1.58370 factor:1 | 1 (-1.66574) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.06792 HOMO: -6.87087 LUMO: -0.82995 factor:1 | 1 (-2.26693) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.76654 HOMO: -6.67223 LUMO: 1.08029 factor:1 | 1 (-2.96555) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.51235 HOMO: -6.82462 LUMO: 0.91702 factor:1 | 1 (-0.71136) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.64184 HOMO: -6.65863 LUMO: 1.52656 factor:1 | 1 (-1.84085) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.89940 HOMO: -6.78924 LUMO: 0.86260 factor:1 | 1 (-2.09841) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.75738 HOMO: -6.68584 LUMO: 0.94424 factor:1 | 1 (-1.95639) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.12359 HOMO: -6.58788 LUMO: 1.00138 factor:1 | 1 (-2.32260) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.65166 HOMO: -6.79740 LUMO: 0.91430 factor:1 | 1 (-1.85067) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.29543 HOMO: -6.67223 LUMO: 0.80274 factor:1 | 1 (-2.49444) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.49222 HOMO: -6.95251 LUMO: 0.90614 factor:1 | 1 (-2.69123) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.93632 HOMO: -7.19469 LUMO: 1.34152 factor:1 | 1 (-2.13533) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.27733 HOMO: -6.59332 LUMO: -0.76464 factor:1 | 1 (-0.47634) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.30535 HOMO: -6.77564 LUMO: -0.90886 factor:1 | 1 (-0.50436) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.49376 HOMO: -6.57971 LUMO: -0.41633 factor:1 | 1 (-0.69277) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.74166 HOMO: -6.68856 LUMO: -0.58232 factor:1 | 1 (-0.94067) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.45967 HOMO: -6.87087 LUMO: -0.71022 factor:1 | 1 (-0.65868) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.37950 HOMO: -6.67767 LUMO: -0.74559 factor:1 | 1 (-0.57851) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.25047 HOMO: -6.68040 LUMO: -0.65307 factor:1 | 1 (-0.44948) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.40574 HOMO: -6.32937 LUMO: 0.80274 factor:1 | 1 (-0.60475) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.89937 HOMO: -6.29671 LUMO: 0.82723 factor:1 | 1 (-2.09838) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.63946 HOMO: -6.67767 LUMO: 0.59321 factor:1 | 1 (-2.83847) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.91014 HOMO: -6.77836 LUMO: 0.50341 factor:1 | 1 (-2.10915) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.94982 HOMO: -6.61781 LUMO: 0.42450 factor:1 | 1 (-2.14883) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.40753 HOMO: -6.83278 LUMO: 0.39457 factor:1 | 1 (-0.60654) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.53783 HOMO: -6.56883 LUMO: 0.64219 factor:1 | -1 (0.26316) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.89415 HOMO: -6.71577 LUMO: 0.40001 factor:1 | 1 (-1.09316) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.50693 HOMO: -6.86543 LUMO: -0.74287 factor:1 | 1 (-0.70594) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.58332 HOMO: -6.68584 LUMO: -0.69389 factor:1 | 1 (-0.78233) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.30865 HOMO: -6.61237 LUMO: -0.48980 factor:1 | 1 (-0.50766) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.53289 HOMO: -6.80285 LUMO: -0.58232 factor:1 | 1 (-0.73190) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.23647 HOMO: -6.88992 LUMO: -0.70205 factor:1 | -1 (1.56452) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.07339 HOMO: -6.95251 LUMO: -0.71838 factor:1 | 1 (-1.27240) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.85646 HOMO: -7.52123 LUMO: 0.27211 factor:1 | 1 (-1.05548) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.43960 HOMO: -6.76747 LUMO: -0.74015 factor:1 | 1 (-1.63862) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.07034 HOMO: -6.55250 LUMO: -0.49797 factor:1 | 1 (-2.26935) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.43569 HOMO: -6.50896 LUMO: -0.46804 factor:1 | 1 (-1.63470) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.21664 HOMO: -7.45320 LUMO: 0.08436 factor:1 | 1 (-0.41565) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.24002 HOMO: -6.82462 LUMO: -0.70477 factor:1 | 1 (-0.43903) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.85029 HOMO: -6.57155 LUMO: -0.43538 factor:1 | 1 (-1.04930) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.24442 HOMO: -6.72665 LUMO: -0.55239 factor:1 | 1 (-1.44343) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.28385 HOMO: -7.05319 LUMO: -1.08573 factor:1 | -1 (1.51714) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.98486 HOMO: -6.56067 LUMO: -0.45715 factor:1 | 1 (-0.18387) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.92592 HOMO: -6.76475 LUMO: -0.53879 factor:1 | 1 (-0.12493) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.12716 HOMO: -6.67223 LUMO: -0.45987 factor:1 | 1 (-1.32617) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.06368 HOMO: -6.44094 LUMO: -0.72110 factor:1 | 1 (-1.26269) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.59322 HOMO: -6.66951 LUMO: -0.67756 factor:1 | 1 (-0.79223) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.75031 HOMO: -6.69400 LUMO: -0.62858 factor:1 | 1 (-0.94932) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.86817 HOMO: -6.51985 LUMO: -0.37007 factor:1 | 1 (-1.06718) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.61154 HOMO: -5.98378 LUMO: 0.78641 factor:1 | 1 (-0.81055) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.43561 HOMO: -6.11440 LUMO: 0.71294 factor:1 | 1 (-0.63462) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.47172 HOMO: -6.45182 LUMO: 0.63947 factor:1 | 1 (-0.67073) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.64727 HOMO: -6.78924 LUMO: 0.37007 factor:1 | -1 (0.15372) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.04613 HOMO: -6.63686 LUMO: 0.54423 factor:1 | 1 (-1.24514) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.95560 HOMO: -6.66679 LUMO: 0.48708 factor:1 | 1 (-1.15461) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.17700 HOMO: -6.81917 LUMO: 0.31021 factor:1 | 1 (-0.37601) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.09797 HOMO: -6.28583 LUMO: 0.44899 factor:1 | 1 (-1.29698) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.36108 HOMO: -6.61237 LUMO: 0.49525 factor:1 | 1 (-0.56009) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.44691 HOMO: -7.08857 LUMO: 0.38368 factor:1 | 1 (-0.64592) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.84754 HOMO: -6.53890 LUMO: -0.68845 factor:1 | 1 (-1.04655) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.81399 HOMO: -6.56611 LUMO: -0.66396 factor:1 | 1 (-1.01300) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.70977 HOMO: -6.04909 LUMO: -0.59865 factor:1 | 1 (-0.90878) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.41242 HOMO: -6.74842 LUMO: -0.77825 factor:1 | 1 (-1.61143) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.42337 HOMO: -6.82462 LUMO: -0.61498 factor:1 | 1 (-0.62238) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.30758 HOMO: -7.40694 LUMO: 0.32926 factor:1 | 1 (-0.50659) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.03727 HOMO: -6.80557 LUMO: -0.57416 factor:1 | 1 (-0.23628) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.87095 HOMO: -6.76747 LUMO: -0.67484 factor:1 | 1 (-0.06996) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.01298 HOMO: -7.23279 LUMO: 0.48980 factor:1 | 1 (-2.21199) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.01231 HOMO: -6.62869 LUMO: -0.24762 factor:1 | 1 (-0.21132) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.18094 HOMO: -6.65863 LUMO: -0.28028 factor:1 | 1 (-0.37995) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.34257 HOMO: -6.50352 LUMO: -0.44899 factor:1 | 1 (-1.54158) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.40009 HOMO: -6.62053 LUMO: -0.88437 factor:1 | 1 (-1.59910) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.93986 HOMO: -6.73754 LUMO: -0.77825 factor:1 | 1 (-2.13887) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.98468 HOMO: -7.24639 LUMO: 0.35647 factor:1 | 1 (-1.18370) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.14836 HOMO: -6.46270 LUMO: -0.48164 factor:1 | 1 (-1.34737) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.95734 HOMO: -6.14161 LUMO: -0.66396 factor:1 | 1 (-1.15635) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.96158 HOMO: -6.63414 LUMO: 1.51295 factor:1 | 1 (-1.16059) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.06177 HOMO: -6.52529 LUMO: 1.65989 factor:1 | 1 (-1.26079) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.63756 HOMO: -6.63686 LUMO: 1.64629 factor:1 | -1 (0.16343) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.58234 HOMO: -6.49808 LUMO: 1.60003 factor:1 | 1 (-0.78135) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.93402 HOMO: -6.85183 LUMO: 1.96194 factor:1 | 1 (-1.13303) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.87914 HOMO: -6.90081 LUMO: 1.82316 factor:1 | 1 (-0.07815) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.95584 HOMO: -6.20147 LUMO: 1.95106 factor:1 | 1 (-1.15485) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.79516 HOMO: -7.05047 LUMO: 1.94289 factor:1 | 1 (-0.99417) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.50435 HOMO: -6.11440 LUMO: 1.83949 factor:1 | 1 (-0.70336) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.12183 HOMO: -6.65046 LUMO: 1.59187 factor:1 | 1 (-1.32084) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.34846 HOMO: -6.81917 LUMO: 2.41365 factor:1 | 1 (-0.54747) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.86047 HOMO: -6.40284 LUMO: 2.48984 factor:1 | 1 (-1.05948) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.46097 HOMO: -7.04775 LUMO: 2.31025 factor:1 | 1 (-0.65998) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.54390 HOMO: -6.64774 LUMO: 2.20140 factor:1 | -1 (0.25709) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.82180 HOMO: -6.72393 LUMO: 2.28304 factor:1 | 1 (-1.02081) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.18991 HOMO: -6.35114 LUMO: 1.84765 factor:1 | 1 (-1.38892) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.94196 HOMO: -6.41100 LUMO: 1.74697 factor:1 | 1 (-1.14097) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.84199 HOMO: -6.34297 LUMO: 1.55921 factor:1 | 1 (-1.04100) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.86655 HOMO: -6.31848 LUMO: 1.67622 factor:1 | 1 (-2.06556) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.73531 HOMO: -6.50896 LUMO: 2.02725 factor:1 | 1 (-1.93432) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.41762 HOMO: -6.28583 LUMO: 2.00548 factor:1 | 1 (-1.61663) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.93082 HOMO: -6.67495 LUMO: 1.92384 factor:1 | 1 (-2.12984) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.58087 HOMO: -6.17154 LUMO: 2.39732 factor:1 | 1 (-0.77988) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.96947 HOMO: -6.84911 LUMO: 2.24766 factor:1 | 1 (-1.16848) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.05260 HOMO: -6.77564 LUMO: 2.38372 factor:1 | 1 (-1.25161) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.15174 HOMO: -6.18243 LUMO: 2.40821 factor:1 | 1 (-1.35075) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.00245 HOMO: -6.40828 LUMO: 2.22589 factor:1 | 1 (-1.20146) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.86403 HOMO: -6.74570 LUMO: 1.88303 factor:1 | 1 (-1.06304) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.65306 HOMO: -6.29944 LUMO: 2.05174 factor:1 | 1 (-0.85207) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.65894 HOMO: -7.00693 LUMO: 2.16331 factor:1 | 1 (-0.85795) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.43906 HOMO: -6.89537 LUMO: 2.19596 factor:1 | 1 (-1.63807) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.73399 HOMO: -6.72665 LUMO: 2.03813 factor:1 | 1 (-0.93300) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.60743 HOMO: -6.69944 LUMO: 2.36467 factor:1 | 1 (-0.80644) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.04612 HOMO: -6.92802 LUMO: 1.72792 factor:1 | 1 (-2.24513) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.61954 HOMO: -6.12256 LUMO: 1.85310 factor:1 | 1 (-0.81855) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.38692 HOMO: -6.70489 LUMO: 2.20956 factor:1 | 1 (-1.58593) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.33519 HOMO: -6.94707 LUMO: 1.81500 factor:1 | 1 (-1.53421) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.80841 HOMO: -6.39468 LUMO: 1.79051 factor:1 | 1 (-1.00742) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.72272 HOMO: -6.69128 LUMO: 2.03813 factor:1 | 1 (-0.92173) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.43384 HOMO: -6.55250 LUMO: 2.00548 factor:1 | 1 (-0.63286) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.54245 HOMO: -6.24773 LUMO: 2.09256 factor:1 | 1 (-0.74146) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.39013 HOMO: -6.85727 LUMO: 1.70071 factor:1 | 1 (-1.58914) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.58460 HOMO: -6.71305 LUMO: 1.72520 factor:1 | 1 (-0.78361) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.34045 HOMO: -6.81101 LUMO: 2.15514 factor:1 | 1 (-1.53946) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.71063 HOMO: -6.93618 LUMO: 1.75513 factor:1 | 1 (-1.90964) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.37660 HOMO: -6.63686 LUMO: 2.09800 factor:1 | 1 (-2.57561) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.20442 HOMO: -6.98244 LUMO: 1.72520 factor:1 | 1 (-1.40343) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.40325 HOMO: -6.37019 LUMO: 2.35923 factor:1 | 1 (-1.60226) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.97156 HOMO: -6.55794 LUMO: 2.12521 factor:1 | 1 (-2.17057) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.50037 HOMO: -6.45998 LUMO: 1.93201 factor:1 | 1 (-1.69938) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.68176 HOMO: -6.71033 LUMO: 1.58370 factor:1 | 1 (-1.88077) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.08906 HOMO: -6.67223 LUMO: 1.52928 factor:1 | 1 (-2.28807) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.45860 HOMO: -6.72121 LUMO: 1.33608 factor:1 | 1 (-1.65761) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.99009 HOMO: -6.89264 LUMO: 2.08983 factor:1 | 1 (-2.18910) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.34388 HOMO: -6.31032 LUMO: 2.24766 factor:1 | 1 (-1.54289) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.42087 HOMO: -6.79740 LUMO: 2.09528 factor:1 | 1 (-0.61988) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.97428 HOMO: -6.78108 LUMO: 2.15786 factor:1 | 1 (-2.17329) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.53718 HOMO: -6.50896 LUMO: 2.15786 factor:1 | 1 (-1.73620) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.09969 HOMO: -6.56067 LUMO: 2.24494 factor:1 | 1 (-0.29870) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.55261 HOMO: -6.72938 LUMO: 2.24494 factor:1 | 1 (-1.75162) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.09209 HOMO: -6.40556 LUMO: 1.58642 factor:1 | 1 (-1.29110) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.36595 HOMO: -6.63141 LUMO: 1.66262 factor:1 | 1 (-0.56496) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.31794 HOMO: -6.97156 LUMO: 2.23678 factor:1 | 1 (-1.51695) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.91257 HOMO: -6.86271 LUMO: 1.91296 factor:1 | 1 (-2.11158) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.75773 HOMO: -6.50624 LUMO: 1.89119 factor:1 | 1 (-1.95674) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.88769 HOMO: -6.70761 LUMO: 1.56193 factor:1 | 1 (-3.08670) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.94038 HOMO: -6.60420 LUMO: 1.79595 factor:1 | 1 (-1.13940) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.01480 HOMO: -6.85727 LUMO: 2.26943 factor:1 | 1 (-2.21381) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.86707 HOMO: -6.23413 LUMO: 1.91024 factor:1 | 1 (-2.06608) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.22436 HOMO: -6.84366 LUMO: 2.01364 factor:1 | 1 (-1.42337) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.82591 HOMO: -6.63414 LUMO: 2.54971 factor:1 | 1 (-1.02492) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.84666 HOMO: -6.52257 LUMO: 2.42998 factor:1 | 1 (-2.04567) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.26374 HOMO: -6.61509 LUMO: 2.31297 factor:1 | 1 (-1.46275) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.90719 HOMO: -6.45998 LUMO: 2.23405 factor:1 | 1 (-1.10620) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.62058 HOMO: -6.86271 LUMO: 2.22317 factor:1 | 1 (-2.81959) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.75425 HOMO: -6.84366 LUMO: 2.11432 factor:1 | 1 (-1.95326) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.17586 HOMO: -6.85999 LUMO: 2.44902 factor:1 | 1 (-2.37487) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.50848 HOMO: -6.73482 LUMO: 1.93745 factor:1 | 1 (-1.70749) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.28684 HOMO: -6.91441 LUMO: 2.32385 factor:1 | 1 (-1.48585) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.87091 HOMO: -6.16066 LUMO: 2.26399 factor:1 | 1 (-1.06992) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.09750 HOMO: -6.71305 LUMO: 2.38644 factor:1 | 1 (-1.29651) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.85061 HOMO: -7.08312 LUMO: 2.01636 factor:1 | 1 (-2.04962) | 1 | 1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.53944 HOMO: -6.15249 LUMO: 1.90752 factor:1 | 1 (-1.73845) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.46743 HOMO: -6.83006 LUMO: 2.25855 factor:1 | 1 (-2.66644) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.83100 HOMO: -6.77836 LUMO: 2.24766 factor:1 | 1 (-3.03002) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.37660 HOMO: -6.66951 LUMO: 2.35923 factor:1 | 1 (-2.57561) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.93999 HOMO: -6.68312 LUMO: 2.30208 factor:1 | 1 (-3.13900) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.78208 HOMO: -6.49808 LUMO: 2.49801 factor:1 | 1 (-2.98109) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.26814 HOMO: -6.62325 LUMO: 1.89935 factor:1 | 1 (-2.46715) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.11703 HOMO: -6.80829 LUMO: 1.91296 factor:1 | 1 (-2.31604) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.33829 HOMO: -6.64230 LUMO: 2.13065 factor:1 | 1 (-2.53730) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.24855 HOMO: -6.40556 LUMO: 1.83949 factor:1 | 1 (-2.44756) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.48407 HOMO: -6.48175 LUMO: 1.72248 factor:1 | 1 (-1.68308) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.43525 HOMO: -6.61781 LUMO: 2.11432 factor:1 | 1 (-1.63426) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.63675 HOMO: -6.34570 LUMO: 2.22317 factor:1 | 1 (-1.83576) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.08607 HOMO: -7.00149 LUMO: 1.80139 factor:1 | 1 (-2.28508) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.24640 HOMO: -6.66951 LUMO: 2.13065 factor:1 | 1 (-2.44541) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.64029 HOMO: -6.54434 LUMO: 2.20140 factor:1 | 1 (-1.83930) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.24050 HOMO: -6.67767 LUMO: 2.02997 factor:1 | 1 (-1.43951) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.38094 HOMO: -6.49536 LUMO: 2.42998 factor:1 | 1 (-1.57995) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.59122 HOMO: -6.70761 LUMO: 2.71025 factor:1 | 1 (-2.79023) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.48957 HOMO: -6.62869 LUMO: 2.11160 factor:1 | 1 (-1.68858) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.10400 HOMO: -6.61781 LUMO: 2.24494 factor:1 | 1 (-2.30301) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.70606 HOMO: -6.66135 LUMO: 2.20956 factor:1 | 1 (-1.90507) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.87353 HOMO: -6.95523 LUMO: 2.03813 factor:1 | 1 (-1.07254) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.84372 HOMO: -7.11578 LUMO: 2.41365 factor:1 | 1 (-2.04273) | 1 | 1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.52930 HOMO: -6.99061 LUMO: 2.13881 factor:1 | 1 (-0.72831) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.23852 HOMO: -6.43277 LUMO: 2.01364 factor:1 | 1 (-0.43753) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.33861 HOMO: -6.79196 LUMO: 2.04358 factor:1 | 1 (-0.53762) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.51624 HOMO: -7.08584 LUMO: 1.99732 factor:1 | 1 (-0.71525) | 1 | 1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.76348 HOMO: -6.46815 LUMO: 2.29936 factor:1 | 1 (-0.96249) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.31261 HOMO: -6.78108 LUMO: 1.93745 factor:1 | 1 (-1.51162) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.52579 HOMO: -6.43277 LUMO: 1.80956 factor:1 | 1 (-0.72480) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.60797 HOMO: -6.71577 LUMO: -0.81090 factor:1 | 1 (-0.80698) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.36767 HOMO: -7.14027 LUMO: -0.68028 factor:1 | 1 (-0.56668) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.40086 HOMO: -7.03414 LUMO: -0.69661 factor:1 | 1 (-0.59988) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.71110 HOMO: -6.64502 LUMO: -0.47348 factor:1 | 1 (-0.91011) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.67736 HOMO: -6.60692 LUMO: 2.12793 factor:1 | 1 (-0.87637) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.43482 HOMO: -6.66407 LUMO: 1.94561 factor:1 | 1 (-1.63383) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.08803 HOMO: -7.10217 LUMO: 1.92384 factor:1 | 1 (-1.28704) | 1 | 1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.89558 HOMO: -6.84094 LUMO: 1.66534 factor:1 | 1 (-3.09459) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.81588 HOMO: -6.93618 LUMO: 2.13065 factor:1 | 1 (-2.01489) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.27081 HOMO: -6.60692 LUMO: 2.20684 factor:1 | 1 (-1.46982) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.58685 HOMO: -6.85727 LUMO: 2.19324 factor:1 | 1 (-1.78586) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.28238 HOMO: -6.31032 LUMO: 1.76330 factor:1 | 1 (-1.48139) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.90226 HOMO: -6.43821 LUMO: 2.10072 factor:1 | 1 (-1.10127) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.67053 HOMO: -6.42189 LUMO: 2.19596 factor:1 | 1 (-0.86954) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.00769 HOMO: -6.40556 LUMO: 2.02181 factor:1 | 1 (-0.20670) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.15955 HOMO: -6.41372 LUMO: 2.26671 factor:1 | 1 (-0.35856) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.62819 HOMO: -6.60692 LUMO: 2.09800 factor:1 | 1 (-0.82720) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.48647 HOMO: -6.75931 LUMO: 1.76602 factor:1 | 1 (-0.68548) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.87608 HOMO: -6.39195 LUMO: 1.84221 factor:1 | 1 (-1.07509) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.76185 HOMO: -6.74570 LUMO: 2.04085 factor:1 | 1 (-0.96086) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.97182 HOMO: -6.77019 LUMO: 2.16875 factor:1 | 1 (-0.17083) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.04347 HOMO: -6.15522 LUMO: 1.81772 factor:1 | 1 (-0.24248) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.30562 HOMO: -6.48175 LUMO: 2.02453 factor:1 | 1 (-0.50464) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.08831 HOMO: -6.57427 LUMO: 1.77962 factor:1 | 1 (-0.28733) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.73761 HOMO: -6.57699 LUMO: 2.42998 factor:1 | 1 (-0.93662) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.56038 HOMO: -6.35386 LUMO: 2.25310 factor:1 | 1 (-0.75939) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.41828 HOMO: -6.80013 LUMO: 2.11160 factor:1 | 1 (-0.61729) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.54963 HOMO: -6.24229 LUMO: 2.05718 factor:1 | 1 (-0.74864) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.63306 HOMO: -6.42733 LUMO: 1.76874 factor:1 | 1 (-0.83207) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.99919 HOMO: -6.56883 LUMO: 2.36195 factor:1 | 1 (-1.19820) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.82221 HOMO: -6.72665 LUMO: 2.28848 factor:1 | 1 (-1.02122) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.57491 HOMO: -6.39195 LUMO: 1.79051 factor:1 | 1 (-0.77392) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.47395 HOMO: -6.70761 LUMO: 0.15510 factor:1 | 1 (-1.67296) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.76035 HOMO: -6.44366 LUMO: -0.16871 factor:1 | 1 (-1.95936) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.89186 HOMO: -6.68584 LUMO: 1.69527 factor:1 | 1 (-2.09087) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.05636 HOMO: -6.26950 LUMO: 1.61636 factor:1 | 1 (-1.25537) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.24665 HOMO: -6.47631 LUMO: 1.98915 factor:1 | 1 (-1.44566) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.87926 HOMO: -6.58243 LUMO: 1.97283 factor:1 | 1 (-2.07827) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.45876 HOMO: -6.51713 LUMO: 1.97283 factor:1 | 1 (-1.65777) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.56064 HOMO: -6.65046 LUMO: 1.69255 factor:1 | 1 (-1.75965) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.79347 HOMO: -6.26406 LUMO: 2.21773 factor:1 | 1 (-0.99248) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.14157 HOMO: -6.88992 LUMO: 2.28304 factor:1 | 1 (-0.34058) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.06570 HOMO: -6.67767 LUMO: 2.34834 factor:1 | 1 (-0.26471) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.02172 HOMO: -6.52801 LUMO: 2.10344 factor:1 | 1 (-1.22073) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.39547 HOMO: -6.52801 LUMO: 2.24222 factor:1 | 1 (-1.59448) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.77112 HOMO: -6.17154 LUMO: 1.89663 factor:1 | 1 (-1.97013) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.09309 HOMO: -6.42733 LUMO: 2.15514 factor:1 | 1 (-2.29210) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.98160 HOMO: -6.36474 LUMO: 2.01364 factor:1 | 1 (-2.18061) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.56611 HOMO: -6.82189 LUMO: 1.86942 factor:1 | 1 (-1.76512) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.35046 HOMO: -6.60148 LUMO: 2.00548 factor:1 | 1 (-1.54947) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.21644 HOMO: -6.67767 LUMO: 2.15786 factor:1 | 1 (-2.41545) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.97308 HOMO: -6.79196 LUMO: 2.06534 factor:1 | 1 (-3.17209) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.95063 HOMO: -6.70216 LUMO: 1.83405 factor:1 | 1 (-2.14965) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.15963 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-1.35864) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.16189 HOMO: -6.34842 LUMO: 1.80139 factor:1 | 1 (-1.36090) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.28834 HOMO: -6.48175 LUMO: 1.95922 factor:1 | 1 (-1.48735) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.73839 HOMO: -6.71033 LUMO: 2.02997 factor:1 | 1 (-0.93741) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.77641 HOMO: -6.89264 LUMO: 2.42726 factor:1 | 1 (-0.97542) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.51309 HOMO: -6.74570 LUMO: 2.20684 factor:1 | 1 (-2.71210) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.17815 HOMO: -6.30216 LUMO: 2.15242 factor:1 | 1 (-2.37716) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.98756 HOMO: -6.94979 LUMO: 2.43814 factor:1 | 1 (-2.18657) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.00277 HOMO: -6.97972 LUMO: 2.11432 factor:1 | 1 (-2.20178) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.40352 HOMO: -6.17154 LUMO: 1.98099 factor:1 | 1 (-1.60253) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.39182 HOMO: -6.74026 LUMO: 2.21501 factor:1 | 1 (-1.59083) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.11742 HOMO: -6.72393 LUMO: 2.19596 factor:1 | 1 (-1.31643) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.33220 HOMO: -6.11440 LUMO: 2.10072 factor:1 | 1 (-1.53121) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.17699 HOMO: -6.34297 LUMO: 1.92657 factor:1 | 1 (-1.37600) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.49699 HOMO: -6.24773 LUMO: 2.00276 factor:1 | 1 (-1.69600) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.35612 HOMO: -6.75114 LUMO: 1.98643 factor:1 | 1 (-1.55513) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.59300 HOMO: -6.69128 LUMO: 2.08711 factor:1 | 1 (-0.79201) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.17802 HOMO: -6.65318 LUMO: 2.15514 factor:1 | 1 (-1.37703) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.91905 HOMO: -6.67495 LUMO: 1.72248 factor:1 | 1 (-1.11806) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.36593 HOMO: -6.58243 LUMO: 1.83405 factor:1 | 1 (-0.56494) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.30742 HOMO: -6.61237 LUMO: 1.69799 factor:1 | 1 (-0.50643) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.10082 HOMO: -6.57427 LUMO: 2.29936 factor:1 | 1 (-1.29983) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.93747 HOMO: -6.40012 LUMO: 2.35378 factor:1 | 1 (-1.13648) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.97808 HOMO: -6.90081 LUMO: 2.26671 factor:1 | 1 (-0.17709) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.75023 HOMO: -6.44910 LUMO: 2.25855 factor:1 | 1 (-0.94924) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.01250 HOMO: -6.61509 LUMO: 2.26943 factor:1 | 1 (-1.21151) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.10910 HOMO: -6.78924 LUMO: 2.09256 factor:1 | 1 (-1.30811) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.27919 HOMO: -6.47087 LUMO: 1.97555 factor:1 | 1 (-1.47820) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.69888 HOMO: -6.75931 LUMO: 1.98643 factor:1 | 1 (-0.89789) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.83674 HOMO: -6.17971 LUMO: 2.09800 factor:1 | 1 (-1.03575) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.31357 HOMO: -6.83006 LUMO: 1.91840 factor:1 | 1 (-0.51258) | -1 | -1 |
| G: -6153.43530 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.40484 HOMO: -6.72938 LUMO: 2.17419 factor:1 | 1 (-0.60385) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.87518 HOMO: -6.78924 LUMO: 2.42726 factor:1 | -1 (1.90703) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.88217 HOMO: -6.41372 LUMO: 1.93745 factor:1 | -1 (1.90004) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.07427 HOMO: -6.85455 LUMO: 2.14970 factor:1 | -1 (0.70793) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.87217 HOMO: -6.38651 LUMO: 2.18507 factor:1 | 1 (-0.08996) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.84066 HOMO: -6.81373 LUMO: 2.00548 factor:1 | 1 (-0.05845) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.85009 HOMO: -6.64774 LUMO: 2.41365 factor:1 | -1 (1.93212) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.31411 HOMO: -6.70489 LUMO: 2.31569 factor:1 | -1 (0.46809) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.84819 HOMO: -6.49264 LUMO: 1.78779 factor:1 | 1 (-0.06599) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.80150 HOMO: -6.81101 LUMO: 1.86670 factor:1 | 1 (-0.01929) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.52938 HOMO: -6.72121 LUMO: 1.48846 factor:1 | -1 (0.25282) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.65359 HOMO: -6.35930 LUMO: 1.78507 factor:1 | -1 (1.12862) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.54319 HOMO: -6.38651 LUMO: 2.04358 factor:1 | -1 (1.23902) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.51995 HOMO: -6.42189 LUMO: 1.99187 factor:1 | -1 (1.26225) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.32395 HOMO: -6.69400 LUMO: 1.61091 factor:1 | -1 (1.45826) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.59485 HOMO: -6.81101 LUMO: 2.17419 factor:1 | -1 (0.18735) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.74863 HOMO: -6.90897 LUMO: 2.28576 factor:1 | -1 (1.03357) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.74751 HOMO: -6.75387 LUMO: 2.31297 factor:1 | -1 (0.03469) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.90411 HOMO: -7.05863 LUMO: 2.18780 factor:1 | 1 (-0.12191) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.10181 HOMO: -6.56611 LUMO: 1.99187 factor:1 | -1 (0.68039) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.26620 HOMO: -6.59060 LUMO: 1.86398 factor:1 | -1 (1.51600) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.16764 HOMO: -6.59060 LUMO: 1.59459 factor:1 | -1 (1.61456) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.77200 HOMO: -6.57699 LUMO: 1.48030 factor:1 | -1 (0.01020) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.83295 HOMO: -6.99605 LUMO: 2.30208 factor:1 | 1 (-0.05075) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.38723 HOMO: -6.42189 LUMO: 2.20412 factor:1 | -1 (0.39497) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.35103 HOMO: -7.15115 LUMO: 1.83405 factor:1 | -1 (2.43117) | 1 | 1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.21513 HOMO: -7.08040 LUMO: 2.21773 factor:1 | -1 (1.56708) | 1 | 1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.41683 HOMO: -6.72121 LUMO: 1.89663 factor:1 | -1 (2.36538) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.65989 HOMO: -6.25590 LUMO: 1.85037 factor:1 | -1 (0.12232) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.99869 HOMO: -6.70489 LUMO: 1.98915 factor:1 | -1 (1.78352) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.50955 HOMO: -6.53617 LUMO: 2.08439 factor:1 | -1 (0.27266) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.55601 HOMO: -6.69944 LUMO: 1.98915 factor:1 | -1 (1.22620) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.08329 HOMO: -6.79468 LUMO: 1.96466 factor:1 | -1 (1.69892) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.07118 HOMO: -6.79468 LUMO: 1.99459 factor:1 | -1 (1.71102) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.70677 HOMO: -6.58788 LUMO: 1.98371 factor:1 | -1 (2.07544) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.60643 HOMO: -6.58788 LUMO: 2.16603 factor:1 | -1 (1.17578) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.75052 HOMO: -6.56883 LUMO: 1.64085 factor:1 | -1 (2.03168) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12414.84417 HOMO: -7.19197 LUMO: 2.66127 factor:1 | -1 (3.93803) | 1 | 1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.77580 HOMO: -6.48175 LUMO: 2.40004 factor:1 | -1 (2.00640) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.30284 HOMO: -6.18515 LUMO: 2.27759 factor:1 | -1 (2.47937) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.56772 HOMO: -6.64774 LUMO: 2.13337 factor:1 | -1 (2.21449) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.45343 HOMO: -6.39740 LUMO: 1.95106 factor:1 | -1 (2.32878) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12414.78776 HOMO: -6.59332 LUMO: 1.81772 factor:1 | -1 (3.99444) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.69659 HOMO: -6.68312 LUMO: 2.41909 factor:1 | -1 (2.08562) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.77841 HOMO: -5.87494 LUMO: 2.18235 factor:1 | -1 (2.00379) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.72726 HOMO: -6.30488 LUMO: 2.04902 factor:1 | -1 (2.05495) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12414.96322 HOMO: -6.65046 LUMO: 2.05446 factor:1 | -1 (3.81898) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.10646 HOMO: -6.55794 LUMO: 2.06807 factor:1 | -1 (2.67575) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.49272 HOMO: -6.68040 LUMO: 1.99187 factor:1 | -1 (2.28948) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.59144 HOMO: -6.60965 LUMO: 2.18780 factor:1 | -1 (2.19076) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12414.36297 HOMO: -6.88176 LUMO: 2.10344 factor:1 | -1 (4.41924) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.21822 HOMO: -6.63414 LUMO: 1.70615 factor:1 | -1 (0.56398) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.35857 HOMO: -7.15115 LUMO: 2.07351 factor:1 | 1 (-0.57636) | 1 | 1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.42163 HOMO: -6.85727 LUMO: 2.27759 factor:1 | -1 (0.36058) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.33519 HOMO: -6.91713 LUMO: 2.28848 factor:1 | 1 (-0.55299) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.48576 HOMO: -7.10217 LUMO: 2.14698 factor:1 | -1 (0.29644) | 1 | 1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.23750 HOMO: -6.78108 LUMO: 2.45447 factor:1 | 1 (-1.45529) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.63931 HOMO: -6.78380 LUMO: 2.43542 factor:1 | 1 (-0.85710) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.66741 HOMO: -6.60965 LUMO: 2.33474 factor:1 | 1 (-1.88520) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.91248 HOMO: -6.72665 LUMO: 2.25855 factor:1 | 1 (-2.13027) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.76267 HOMO: -6.27495 LUMO: 2.04358 factor:1 | -1 (0.01954) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.83619 HOMO: -6.17426 LUMO: 1.45853 factor:1 | 1 (-0.05399) | -1 | -1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.16359 HOMO: -7.21374 LUMO: 2.33474 factor:1 | 1 (-1.38139) | 1 | 1 |
| G: -6154.41651 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.44961 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-1.66740) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.83490 HOMO: -6.80829 LUMO: 0.17960 factor:1 | 1 (-1.05270) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.32219 HOMO: -7.19469 LUMO: 1.60819 factor:1 | 1 (-0.53998) | 1 | 1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.97054 HOMO: -6.78652 LUMO: 0.53334 factor:1 | 1 (-0.18833) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.65096 HOMO: -6.70489 LUMO: 0.74559 factor:1 | 1 (-0.86875) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.40088 HOMO: -6.72393 LUMO: 0.88981 factor:1 | 1 (-0.61868) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.04528 HOMO: -4.54430 LUMO: -0.90614 factor:1 | 1 (-0.26308) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.87690 HOMO: -6.83006 LUMO: 0.47348 factor:1 | 1 (-0.09470) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.36951 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-0.58730) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.73975 HOMO: -6.62053 LUMO: 0.74559 factor:1 | 1 (-0.95754) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.43677 HOMO: -6.79196 LUMO: 1.80139 factor:1 | 1 (-0.65457) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.16125 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-1.37905) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.20208 HOMO: -6.74026 LUMO: 0.95784 factor:1 | 1 (-0.41987) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.34191 HOMO: -7.34707 LUMO: 0.40001 factor:1 | -1 (1.44030) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.32809 HOMO: -6.19875 LUMO: -0.88709 factor:1 | 1 (-0.54589) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.89828 HOMO: -6.48719 LUMO: -0.14694 factor:1 | 1 (-1.11607) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.40110 HOMO: -6.73482 LUMO: -0.01633 factor:1 | 1 (-0.61890) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.31650 HOMO: -7.05591 LUMO: -0.20136 factor:1 | 1 (-0.53430) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.32894 HOMO: -6.38651 LUMO: -2.07895 factor:1 | 1 (-0.54673) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.59589 HOMO: -6.85455 LUMO: -1.03403 factor:1 | -1 (0.18632) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.30815 HOMO: -6.72121 LUMO: -0.99322 factor:1 | 1 (-0.52594) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.09236 HOMO: -6.53890 LUMO: -0.10885 factor:1 | 1 (-0.31016) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.44302 HOMO: -6.68312 LUMO: 0.21225 factor:1 | -1 (0.33919) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.31627 HOMO: -6.68040 LUMO: 0.21225 factor:1 | 1 (-1.53407) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.31630 HOMO: -6.76475 LUMO: -0.64491 factor:1 | 1 (-1.53410) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.10022 HOMO: -6.48175 LUMO: 0.41633 factor:1 | 1 (-1.31801) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.54515 HOMO: -6.42733 LUMO: 0.16599 factor:1 | 1 (-1.76294) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.93077 HOMO: -6.66679 LUMO: 0.77825 factor:1 | 1 (-1.14857) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.86347 HOMO: -6.75931 LUMO: -0.73471 factor:1 | 1 (-2.08126) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.29546 HOMO: -6.53617 LUMO: 0.38096 factor:1 | 1 (-1.51325) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.87560 HOMO: -6.34297 LUMO: 0.35375 factor:1 | 1 (-2.09340) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.47921 HOMO: -7.11850 LUMO: -0.03265 factor:1 | -1 (0.30300) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.17737 HOMO: -5.21914 LUMO: 1.29798 factor:1 | 1 (-0.39516) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.98327 HOMO: -7.09129 LUMO: -0.66668 factor:1 | 1 (-0.20106) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.55344 HOMO: -6.96884 LUMO: -0.31021 factor:1 | -1 (0.22877) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.73384 HOMO: -6.51713 LUMO: -0.59865 factor:1 | 1 (-0.95164) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.74705 HOMO: -6.69400 LUMO: -0.07075 factor:1 | -1 (0.03516) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.54025 HOMO: -5.28173 LUMO: 1.17281 factor:1 | 1 (-1.75805) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.84982 HOMO: -6.54434 LUMO: 0.32109 factor:1 | 1 (-1.06761) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.58107 HOMO: -6.79740 LUMO: -0.24762 factor:1 | 1 (-1.79886) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.71248 HOMO: -6.91986 LUMO: -0.14694 factor:1 | 1 (-0.93028) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.17235 HOMO: -6.75114 LUMO: 0.18504 factor:1 | 1 (-1.39015) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.72208 HOMO: -6.74842 LUMO: 0.69389 factor:1 | -1 (1.06013) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.95228 HOMO: -7.01782 LUMO: 0.56600 factor:1 | 1 (-0.17007) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.01535 HOMO: -6.47359 LUMO: -0.56600 factor:1 | 1 (-0.23315) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.94387 HOMO: -6.63686 LUMO: -0.55783 factor:1 | 1 (-0.16166) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.05453 HOMO: -4.13885 LUMO: -2.05446 factor:1 | 1 (-1.27232) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.84503 HOMO: -6.34570 LUMO: 0.19864 factor:1 | 1 (-1.06282) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.69392 HOMO: -6.47903 LUMO: 0.24762 factor:1 | 1 (-0.91172) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.07129 HOMO: -6.15249 LUMO: 0.32109 factor:1 | 1 (-1.28908) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.40061 HOMO: -6.84366 LUMO: 0.29116 factor:1 | 1 (-0.61841) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.62921 HOMO: -6.34297 LUMO: 0.19864 factor:1 | 1 (-0.84701) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.18253 HOMO: -6.51168 LUMO: 0.30749 factor:1 | 1 (-1.40033) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.45726 HOMO: -6.79468 LUMO: -0.16599 factor:1 | 1 (-1.67505) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.82671 HOMO: -7.24095 LUMO: 0.15238 factor:1 | 1 (-2.04450) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.34076 HOMO: -7.06952 LUMO: -0.34558 factor:1 | 1 (-1.55856) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.77969 HOMO: -6.88176 LUMO: 0.02177 factor:1 | 1 (-0.99749) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.06797 HOMO: -6.37291 LUMO: -0.69117 factor:1 | 1 (-1.28577) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.07151 HOMO: -6.83278 LUMO: -0.59049 factor:1 | 1 (-1.28930) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.14958 HOMO: -6.57155 LUMO: -0.33470 factor:1 | 1 (-1.36737) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.56572 HOMO: -6.89537 LUMO: -0.58504 factor:1 | 1 (-1.78352) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.46958 HOMO: -6.57155 LUMO: -0.34831 factor:1 | 1 (-1.68738) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.99972 HOMO: -6.64774 LUMO: -0.95784 factor:1 | 1 (-1.21752) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.29238 HOMO: -6.91713 LUMO: -0.69933 factor:1 | 1 (-1.51018) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.18776 HOMO: -6.80557 LUMO: -0.65035 factor:1 | 1 (-0.40556) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.79586 HOMO: -7.26544 LUMO: -0.79729 factor:1 | 1 (-1.01365) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.69151 HOMO: -6.69128 LUMO: -0.16871 factor:1 | -1 (0.09070) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.74770 HOMO: -6.88448 LUMO: 0.13061 factor:1 | -1 (0.03450) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.86564 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-2.08344) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.38257 HOMO: -6.56067 LUMO: 0.17687 factor:1 | 1 (-0.60036) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.40821 HOMO: -6.70216 LUMO: 0.25034 factor:1 | -1 (0.37399) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.13865 HOMO: -6.51713 LUMO: -0.78369 factor:1 | 1 (-0.35644) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.03720 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-0.25500) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.23460 HOMO: -6.22052 LUMO: -0.83811 factor:1 | -1 (0.54760) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.39191 HOMO: -6.51168 LUMO: -0.76464 factor:1 | -1 (0.39029) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.83671 HOMO: -7.14571 LUMO: -0.80274 factor:1 | 1 (-0.05450) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.15497 HOMO: -6.66679 LUMO: -0.88709 factor:1 | 1 (-0.37277) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.80302 HOMO: -6.76203 LUMO: -1.43948 factor:1 | 1 (-0.02082) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.15910 HOMO: -6.57427 LUMO: -1.62996 factor:1 | 1 (-1.37690) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.49144 HOMO: -5.05043 LUMO: 1.24900 factor:1 | 1 (-0.70924) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.27682 HOMO: -6.53345 LUMO: 0.23130 factor:1 | 1 (-1.49461) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.78677 HOMO: -7.18381 LUMO: -0.22585 factor:1 | 1 (-1.00456) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.25154 HOMO: -7.00965 LUMO: -1.79595 factor:1 | 1 (-1.46933) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12421.04709 HOMO: -6.08174 LUMO: -0.82995 factor:1 | 1 (-2.26489) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.07515 HOMO: -6.42189 LUMO: -0.84355 factor:1 | 1 (-1.29295) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.60791 HOMO: -6.53890 LUMO: 0.60409 factor:1 | 1 (-0.82570) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.55827 HOMO: -6.62869 LUMO: 0.43810 factor:1 | 1 (-0.77607) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.54790 HOMO: -6.68312 LUMO: 0.64491 factor:1 | 1 (-1.76569) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.25363 HOMO: -6.42189 LUMO: 1.51295 factor:1 | 1 (-1.47143) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.10533 HOMO: -6.17971 LUMO: 1.67622 factor:1 | 1 (-1.32313) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.13344 HOMO: -6.79196 LUMO: 1.36873 factor:1 | 1 (-1.35124) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.78127 HOMO: -7.38517 LUMO: 0.56328 factor:1 | 1 (-0.99907) | 1 | 1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.91485 HOMO: -7.56204 LUMO: 0.71566 factor:1 | 1 (-1.13265) | 1 | 1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.05337 HOMO: -6.45726 LUMO: -1.91840 factor:1 | 1 (-0.27116) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.58105 HOMO: -6.13073 LUMO: -0.97417 factor:1 | 1 (-0.79884) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.18431 HOMO: -6.50352 LUMO: -0.69661 factor:1 | 1 (-0.40210) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.44478 HOMO: -6.76747 LUMO: -1.71976 factor:1 | 1 (-0.66257) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.07043 HOMO: -6.48447 LUMO: -0.89525 factor:1 | 1 (-0.28822) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.85608 HOMO: -7.11850 LUMO: -0.71566 factor:1 | 1 (-0.07388) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.06997 HOMO: -6.80285 LUMO: -0.49253 factor:1 | 1 (-0.28776) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.79886 HOMO: -6.80557 LUMO: -0.88165 factor:1 | 1 (-0.01665) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.53733 HOMO: -6.94162 LUMO: -0.08980 factor:1 | -1 (0.24488) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.60179 HOMO: -6.97972 LUMO: -0.29388 factor:1 | -1 (0.18041) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.77829 HOMO: -6.75114 LUMO: 0.04626 factor:1 | -1 (0.00392) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.98814 HOMO: -7.15932 LUMO: 0.68845 factor:1 | 1 (-0.20594) | 1 | 1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.30297 HOMO: -7.36612 LUMO: 0.63675 factor:1 | 1 (-1.52076) | 1 | 1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.99387 HOMO: -7.02598 LUMO: -0.66124 factor:1 | 1 (-1.21167) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.64995 HOMO: -6.89264 LUMO: -0.54967 factor:1 | 1 (-0.86774) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.39494 HOMO: -6.97700 LUMO: 0.27756 factor:1 | 1 (-1.61274) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.39361 HOMO: -6.60965 LUMO: 0.08163 factor:1 | 1 (-1.61140) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.95427 HOMO: -6.70761 LUMO: 0.40001 factor:1 | 1 (-2.17207) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.29886 HOMO: -6.69128 LUMO: 0.23674 factor:1 | 1 (-1.51665) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.30302 HOMO: -6.69128 LUMO: -0.69933 factor:1 | 1 (-1.52082) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.97895 HOMO: -6.18515 LUMO: -0.85988 factor:1 | 1 (-2.19675) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.63451 HOMO: -6.86815 LUMO: -1.90208 factor:1 | 1 (-1.85231) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.30942 HOMO: -6.37563 LUMO: -1.74697 factor:1 | 1 (-1.52721) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.61288 HOMO: -6.75659 LUMO: 0.36463 factor:1 | 1 (-1.83067) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.01107 HOMO: -6.91441 LUMO: -0.88981 factor:1 | 1 (-1.22887) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.28224 HOMO: -6.71305 LUMO: -0.29933 factor:1 | 1 (-0.50004) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.27786 HOMO: -6.91441 LUMO: -1.04492 factor:1 | 1 (-0.49566) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.96795 HOMO: -6.05453 LUMO: -0.83539 factor:1 | 1 (-0.18574) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.83304 HOMO: -7.35252 LUMO: -0.45715 factor:1 | 1 (-0.05083) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.98569 HOMO: -6.41644 LUMO: -0.97417 factor:1 | 1 (-0.20349) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.82947 HOMO: -6.78924 LUMO: 0.36735 factor:1 | 1 (-0.04727) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.78305 HOMO: -6.74298 LUMO: 0.51974 factor:1 | 1 (-0.00084) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.79540 HOMO: -6.48992 LUMO: 1.44765 factor:1 | 1 (-0.01320) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.67292 HOMO: -6.12528 LUMO: 1.57826 factor:1 | -1 (0.10928) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.63710 HOMO: -6.62325 LUMO: 1.57826 factor:1 | 1 (-1.85489) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.84701 HOMO: -6.19875 LUMO: 1.29798 factor:1 | 1 (-1.06481) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.10375 HOMO: -6.74570 LUMO: 1.52112 factor:1 | 1 (-1.32155) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.25720 HOMO: -6.84094 LUMO: 1.48574 factor:1 | 1 (-1.47499) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.39218 HOMO: -6.85183 LUMO: 0.33470 factor:1 | 1 (-0.60997) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.14016 HOMO: -6.51168 LUMO: 0.48164 factor:1 | 1 (-1.35796) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.69169 HOMO: -6.25046 LUMO: 0.75648 factor:1 | 1 (-0.90949) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.44305 HOMO: -6.65591 LUMO: 0.32109 factor:1 | 1 (-1.66085) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.99513 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-0.21293) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.18088 HOMO: -6.75114 LUMO: 0.73471 factor:1 | 1 (-0.39867) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.51562 HOMO: -6.50624 LUMO: 0.59321 factor:1 | 1 (-1.73342) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.71351 HOMO: -6.39740 LUMO: 0.83267 factor:1 | 1 (-0.93131) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.57449 HOMO: -6.44094 LUMO: 0.65579 factor:1 | 1 (-0.79229) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.94361 HOMO: -6.52257 LUMO: 0.05714 factor:1 | 1 (-1.16141) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.44835 HOMO: -7.10217 LUMO: 0.49797 factor:1 | -1 (0.33386) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.46999 HOMO: -6.83006 LUMO: 0.55783 factor:1 | -1 (1.31221) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.36678 HOMO: -6.99333 LUMO: -0.79457 factor:1 | 1 (-1.58457) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.54997 HOMO: -6.64230 LUMO: 0.32382 factor:1 | 1 (-0.76777) | -1 | -1 |
| G: -6154.41651 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.47264 HOMO: -6.90897 LUMO: 0.30749 factor:1 | 1 (-0.69043) | -1 | -1 |
| G: -6154.41651 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.55436 HOMO: -7.09129 LUMO: 1.33336 factor:1 | -1 (0.22784) | 1 | 1 |
| G: -6154.41651 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.04998 HOMO: -6.66951 LUMO: 1.34424 factor:1 | 1 (-1.26778) | -1 | -1 |
| G: -6154.41651 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.16052 HOMO: -7.02870 LUMO: 1.48574 factor:1 | 1 (-0.37832) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.12726 HOMO: -7.26544 LUMO: 0.32926 factor:1 | 1 (-1.34506) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.11978 HOMO: -6.56067 LUMO: -0.45987 factor:1 | -1 (1.66243) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.12572 HOMO: -6.54434 LUMO: -0.28300 factor:1 | 1 (-0.34352) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.41513 HOMO: -7.19469 LUMO: 0.54695 factor:1 | -1 (1.36707) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.28872 HOMO: -6.47359 LUMO: -0.22041 factor:1 | 1 (-0.50651) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.22945 HOMO: -6.80013 LUMO: 2.08167 factor:1 | 1 (-0.44725) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.98977 HOMO: -6.23957 LUMO: 1.67894 factor:1 | 1 (-0.20757) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.24398 HOMO: -6.75114 LUMO: -0.62858 factor:1 | 1 (-0.46178) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.82879 HOMO: -6.79468 LUMO: -0.64491 factor:1 | 1 (-0.04659) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.88681 HOMO: -6.84911 LUMO: -0.69661 factor:1 | 1 (-0.10460) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.79616 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-0.01396) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.76634 HOMO: -6.92802 LUMO: -0.71022 factor:1 | -1 (0.01586) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.35993 HOMO: -6.72665 LUMO: -0.46804 factor:1 | 1 (-0.57772) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.07467 HOMO: -6.63686 LUMO: -0.23674 factor:1 | 1 (-0.29247) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.18072 HOMO: -7.21102 LUMO: 0.54423 factor:1 | 1 (-0.39851) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.72514 HOMO: -6.63414 LUMO: -0.25034 factor:1 | -1 (0.05706) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.44061 HOMO: -6.70761 LUMO: -0.31837 factor:1 | 1 (-0.65841) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.59989 HOMO: -6.57155 LUMO: 1.76874 factor:1 | -1 (0.18232) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.35830 HOMO: -6.84366 LUMO: 2.04358 factor:1 | 1 (-0.57609) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.09492 HOMO: -6.60420 LUMO: 1.80139 factor:1 | 1 (-0.31271) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.28183 HOMO: -7.03686 LUMO: 2.21229 factor:1 | 1 (-0.49963) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.36037 HOMO: -6.77564 LUMO: 1.97555 factor:1 | 1 (-0.57816) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.95590 HOMO: -6.40012 LUMO: 2.17691 factor:1 | 1 (-0.17369) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.25574 HOMO: -6.80013 LUMO: 2.25582 factor:1 | 1 (-0.47353) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.66800 HOMO: -6.74298 LUMO: 2.31569 factor:1 | -1 (0.11421) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.89349 HOMO: -6.68856 LUMO: 1.85854 factor:1 | 1 (-1.11129) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.19107 HOMO: -6.17971 LUMO: 1.52928 factor:1 | 1 (-1.40887) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.33356 HOMO: -6.54162 LUMO: 1.91840 factor:1 | 1 (-0.55136) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.96479 HOMO: -6.80013 LUMO: -0.55511 factor:1 | 1 (-0.18259) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.92348 HOMO: -7.46953 LUMO: 0.28572 factor:1 | 1 (-1.14127) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.03424 HOMO: -6.61781 LUMO: -0.54967 factor:1 | 1 (-0.25203) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.98711 HOMO: -6.56339 LUMO: -0.47892 factor:1 | 1 (-0.20490) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.05652 HOMO: -6.65591 LUMO: -0.25307 factor:1 | 1 (-0.27432) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.25555 HOMO: -6.62869 LUMO: -0.23402 factor:1 | 1 (-0.47334) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.35601 HOMO: -6.58243 LUMO: -0.19048 factor:1 | 1 (-0.57381) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.42031 HOMO: -7.27632 LUMO: 0.52790 factor:1 | 1 (-0.63811) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.91919 HOMO: -7.21102 LUMO: 0.57688 factor:1 | 1 (-0.13698) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.75128 HOMO: -6.72393 LUMO: -0.53879 factor:1 | 1 (-0.96908) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.49695 HOMO: -7.42054 LUMO: -0.99322 factor:1 | -1 (0.28526) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.26763 HOMO: -6.88992 LUMO: -0.71838 factor:1 | 1 (-0.48542) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.09364 HOMO: -6.88176 LUMO: -0.61226 factor:1 | 1 (-0.31143) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.35743 HOMO: -7.36340 LUMO: -1.04492 factor:1 | 1 (-0.57522) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.42420 HOMO: -6.65863 LUMO: -0.41906 factor:1 | 1 (-0.64200) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.34847 HOMO: -7.15115 LUMO: -0.66396 factor:1 | 1 (-1.56626) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.59556 HOMO: -7.10489 LUMO: -0.64491 factor:1 | -1 (0.18664) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.04903 HOMO: -7.20285 LUMO: 0.47892 factor:1 | 1 (-1.26683) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.77520 HOMO: -6.55794 LUMO: -0.28844 factor:1 | 1 (-0.99300) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.25053 HOMO: -7.19197 LUMO: -0.69661 factor:1 | 1 (-1.46833) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.50720 HOMO: -6.56883 LUMO: -0.32926 factor:1 | 1 (-0.72499) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.16367 HOMO: -6.70761 LUMO: 1.95650 factor:1 | 1 (-1.38147) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.10555 HOMO: -6.60420 LUMO: 1.80684 factor:1 | 1 (-1.32334) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.38967 HOMO: -6.84094 LUMO: 1.64085 factor:1 | 1 (-0.60747) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.82103 HOMO: -6.69128 LUMO: 1.90208 factor:1 | 1 (-1.03882) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.46937 HOMO: -6.75387 LUMO: 1.70343 factor:1 | 1 (-0.68717) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.80780 HOMO: -7.07496 LUMO: 2.10072 factor:1 | 1 (-1.02560) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.18088 HOMO: -6.99877 LUMO: 2.24494 factor:1 | 1 (-0.39867) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.97074 HOMO: -6.63414 LUMO: 2.17691 factor:1 | 1 (-1.18854) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.82144 HOMO: -6.44638 LUMO: 1.78235 factor:1 | 1 (-1.03923) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.04654 HOMO: -6.87632 LUMO: 1.84221 factor:1 | 1 (-0.26433) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.64853 HOMO: -6.85183 LUMO: 1.68711 factor:1 | 1 (-0.86633) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.72208 HOMO: -6.96339 LUMO: 2.26671 factor:1 | -1 (1.06013) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.43487 HOMO: -6.63141 LUMO: 1.96738 factor:1 | 1 (-0.65267) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.36078 HOMO: -6.37019 LUMO: 2.23133 factor:1 | -1 (0.42142) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.80487 HOMO: -7.11034 LUMO: 2.32385 factor:1 | 1 (-0.02267) | 1 | 1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.34793 HOMO: -6.91986 LUMO: 1.65445 factor:1 | 1 (-0.56572) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.42662 HOMO: -7.12938 LUMO: 2.28304 factor:1 | 1 (-1.64441) | 1 | 1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.25010 HOMO: -6.54978 LUMO: 1.92112 factor:1 | 1 (-0.46790) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.99819 HOMO: -6.83006 LUMO: 2.48712 factor:1 | 1 (-2.21599) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.58861 HOMO: -6.97972 LUMO: 1.96738 factor:1 | 1 (-0.80641) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.54445 HOMO: -6.69944 LUMO: 2.06262 factor:1 | 1 (-0.76225) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.79126 HOMO: -6.76747 LUMO: 2.10888 factor:1 | 1 (-1.00905) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.37785 HOMO: -6.91169 LUMO: 2.06534 factor:1 | 1 (-1.59565) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.85732 HOMO: -7.03414 LUMO: 1.93473 factor:1 | 1 (-2.07511) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.89041 HOMO: -7.03142 LUMO: 2.52250 factor:1 | 1 (-2.10820) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.77335 HOMO: -6.34025 LUMO: 2.61229 factor:1 | 1 (-0.99115) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.03654 HOMO: -6.98788 LUMO: 2.28304 factor:1 | 1 (-1.25434) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.76640 HOMO: -6.97700 LUMO: 2.53882 factor:1 | -1 (0.01581) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.55344 HOMO: -6.58788 LUMO: 1.94289 factor:1 | -1 (0.22877) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.49893 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-0.71672) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.92511 HOMO: -6.55250 LUMO: 1.82861 factor:1 | 1 (-1.14291) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.55369 HOMO: -6.45998 LUMO: 1.75786 factor:1 | 1 (-1.77149) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.71025 HOMO: -6.78924 LUMO: 2.33746 factor:1 | 1 (-0.92804) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.83292 HOMO: -6.85727 LUMO: 1.76058 factor:1 | 1 (-1.05071) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.95641 HOMO: -6.70489 LUMO: 1.84493 factor:1 | 1 (-0.17421) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.32532 HOMO: -6.71305 LUMO: 1.53472 factor:1 | 1 (-0.54311) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.75290 HOMO: -6.76747 LUMO: 1.48846 factor:1 | -1 (0.02931) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.86403 HOMO: -6.69128 LUMO: 1.95922 factor:1 | 1 (-0.08182) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.08675 HOMO: -6.67495 LUMO: 2.05446 factor:1 | 1 (-0.30455) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.91029 HOMO: -6.63686 LUMO: 2.25310 factor:1 | 1 (-0.12808) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.73869 HOMO: -6.63958 LUMO: 2.14154 factor:1 | -1 (0.04351) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.89257 HOMO: -6.62597 LUMO: 2.01908 factor:1 | 1 (-1.11036) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.32784 HOMO: -7.07768 LUMO: 2.14154 factor:1 | 1 (-1.54563) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.81137 HOMO: -6.19603 LUMO: 2.01092 factor:1 | 1 (-1.02916) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.33867 HOMO: -6.65046 LUMO: 2.15786 factor:1 | 1 (-1.55646) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.93684 HOMO: -6.92258 LUMO: 2.31841 factor:1 | 1 (-1.15463) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.85096 HOMO: -6.90081 LUMO: 2.19324 factor:1 | 1 (-1.06875) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.33086 HOMO: -6.85455 LUMO: 1.95650 factor:1 | 1 (-1.54865) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.71783 HOMO: -6.57699 LUMO: 1.76058 factor:1 | 1 (-1.93563) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.85942 HOMO: -6.90625 LUMO: 1.97555 factor:1 | 1 (-1.07722) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.76026 HOMO: -6.97428 LUMO: 1.92929 factor:1 | 1 (-1.97805) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.75708 HOMO: -6.61781 LUMO: -0.41906 factor:1 | 1 (-0.97488) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.21995 HOMO: -6.62869 LUMO: -0.81906 factor:1 | 1 (-1.43774) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.23091 HOMO: -7.01237 LUMO: 2.00548 factor:1 | 1 (-1.44871) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.12071 HOMO: -6.85727 LUMO: 2.17691 factor:1 | 1 (-1.33850) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.06610 HOMO: -6.71849 LUMO: 1.58914 factor:1 | 1 (-0.28390) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.02177 HOMO: -7.52395 LUMO: 0.27211 factor:1 | 1 (-0.23957) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.25293 HOMO: -6.96611 LUMO: -0.72654 factor:1 | 1 (-1.47072) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.62795 HOMO: -6.89537 LUMO: -0.68028 factor:1 | 1 (-1.84575) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.92230 HOMO: -6.84911 LUMO: -0.58504 factor:1 | 1 (-2.14009) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.25056 HOMO: -6.79196 LUMO: -0.55783 factor:1 | 1 (-1.46835) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.81732 HOMO: -6.67767 LUMO: 1.79323 factor:1 | 1 (-2.03511) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.77250 HOMO: -6.54434 LUMO: 1.91024 factor:1 | 1 (-1.99030) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.99099 HOMO: -6.62869 LUMO: 1.69799 factor:1 | 1 (-1.20878) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.49271 HOMO: -6.72393 LUMO: 2.12249 factor:1 | 1 (-1.71051) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.07720 HOMO: -6.66407 LUMO: 2.05990 factor:1 | 1 (-0.29500) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.09756 HOMO: -7.00149 LUMO: 1.82044 factor:1 | 1 (-0.31535) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.00743 HOMO: -7.12122 LUMO: 2.16058 factor:1 | 1 (-0.22523) | 1 | 1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.61344 HOMO: -6.63141 LUMO: 2.21229 factor:1 | -1 (0.16877) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.64305 HOMO: -6.37835 LUMO: 2.32113 factor:1 | -1 (0.13916) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.45182 HOMO: -6.99605 LUMO: 2.00548 factor:1 | 1 (-0.66962) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.45045 HOMO: -6.85999 LUMO: 2.39460 factor:1 | 1 (-1.66825) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.60037 HOMO: -6.85727 LUMO: 2.48712 factor:1 | 1 (-0.81816) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.45634 HOMO: -7.04231 LUMO: 2.40277 factor:1 | 1 (-0.67413) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.02215 HOMO: -6.60692 LUMO: 2.26671 factor:1 | 1 (-1.23994) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.93355 HOMO: -6.67495 LUMO: 2.14698 factor:1 | 1 (-0.15135) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.28956 HOMO: -6.73210 LUMO: 2.06807 factor:1 | 1 (-0.50736) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.62529 HOMO: -7.20013 LUMO: 2.02181 factor:1 | 1 (-1.84308) | 1 | 1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.91661 HOMO: -7.18653 LUMO: 2.29936 factor:1 | 1 (-2.13441) | 1 | 1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12421.01582 HOMO: -6.92802 LUMO: 2.36195 factor:1 | 1 (-2.23362) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.08696 HOMO: -6.89537 LUMO: 1.78779 factor:1 | 1 (-1.30476) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.66909 HOMO: -6.96067 LUMO: 2.31297 factor:1 | -1 (0.11312) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.64291 HOMO: -6.91441 LUMO: 2.50345 factor:1 | -1 (0.13930) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.61140 HOMO: -7.17292 LUMO: 2.12521 factor:1 | -1 (0.17081) | 1 | 1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.58473 HOMO: -6.93618 LUMO: 2.35106 factor:1 | -1 (0.19747) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.74925 HOMO: -6.75931 LUMO: 1.61908 factor:1 | -1 (0.03295) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.69509 HOMO: -6.35930 LUMO: 1.23540 factor:1 | 1 (-0.91289) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.56617 HOMO: -6.17971 LUMO: 1.84493 factor:1 | -1 (0.21603) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.15503 HOMO: -6.72665 LUMO: 2.61229 factor:1 | 1 (-0.37282) | -1 | -1 |
| G: -6154.41651 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.30668 HOMO: -6.62869 LUMO: 2.28304 factor:1 | 1 (-0.52447) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.31471 HOMO: -6.58243 LUMO: 0.28028 factor:1 | -1 (0.46749) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.14679 HOMO: -6.79468 LUMO: 0.14966 factor:1 | -1 (0.63541) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.99327 HOMO: -6.63141 LUMO: 0.31021 factor:1 | -1 (0.78894) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.40322 HOMO: -6.81101 LUMO: 0.13878 factor:1 | 1 (-0.62102) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.25295 HOMO: -6.72665 LUMO: 0.65579 factor:1 | 1 (-1.47075) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.12569 HOMO: -6.53073 LUMO: 0.91430 factor:1 | 1 (-1.34348) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.98010 HOMO: -7.19197 LUMO: 1.62996 factor:1 | 1 (-1.19790) | 1 | 1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.54766 HOMO: -6.69400 LUMO: 0.84627 factor:1 | 1 (-0.76546) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.34483 HOMO: -6.76475 LUMO: 0.51974 factor:1 | 1 (-0.56262) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.52034 HOMO: -6.67767 LUMO: 0.52246 factor:1 | 1 (-0.73814) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.74116 HOMO: -6.73210 LUMO: 0.94424 factor:1 | 1 (-0.95896) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.53315 HOMO: -6.97972 LUMO: 0.60409 factor:1 | 1 (-1.75094) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.11791 HOMO: -7.38517 LUMO: 0.73743 factor:1 | 1 (-0.33571) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.53259 HOMO: -6.48992 LUMO: 1.08301 factor:1 | 1 (-0.75038) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.72383 HOMO: -7.18381 LUMO: 1.61908 factor:1 | 1 (-0.94162) | 1 | 1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.02079 HOMO: -6.74842 LUMO: 0.57960 factor:1 | 1 (-1.23858) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.53457 HOMO: -6.67495 LUMO: 0.77280 factor:1 | 1 (-0.75237) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.72415 HOMO: -6.74570 LUMO: 0.77280 factor:1 | 1 (-0.94195) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.88576 HOMO: -6.73754 LUMO: 0.86804 factor:1 | 1 (-1.10356) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.22351 HOMO: -6.66135 LUMO: 0.94424 factor:1 | 1 (-1.44131) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.95425 HOMO: -6.44638 LUMO: 1.00138 factor:1 | 1 (-1.17205) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.31158 HOMO: -6.65591 LUMO: 1.02043 factor:1 | 1 (-0.52937) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.46703 HOMO: -7.17564 LUMO: 0.50069 factor:1 | 1 (-0.68483) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.60924 HOMO: -6.59332 LUMO: 0.79457 factor:1 | 1 (-0.82704) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.65613 HOMO: -6.76747 LUMO: 1.73881 factor:1 | -1 (0.12607) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.60634 HOMO: -7.00421 LUMO: 1.07485 factor:1 | -1 (0.17587) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.71619 HOMO: -6.94979 LUMO: 1.67894 factor:1 | -1 (0.06601) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.34926 HOMO: -6.66135 LUMO: 0.47076 factor:1 | 1 (-0.56706) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.41553 HOMO: -6.74298 LUMO: 1.85037 factor:1 | -1 (0.36667) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.24826 HOMO: -6.65318 LUMO: 0.95240 factor:1 | -1 (0.53394) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.49115 HOMO: -6.63958 LUMO: 0.78097 factor:1 | -1 (0.29105) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.65173 HOMO: -6.11712 LUMO: 0.40001 factor:1 | -1 (0.13048) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.90787 HOMO: -7.08312 LUMO: 0.92519 factor:1 | 1 (-0.12566) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.81431 HOMO: -6.96067 LUMO: 0.54695 factor:1 | 1 (-0.03211) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.43955 HOMO: -6.74026 LUMO: 0.60137 factor:1 | 1 (-0.65735) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.97309 HOMO: -6.74298 LUMO: 0.59593 factor:1 | 1 (-0.19089) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.76933 HOMO: -6.93074 LUMO: 0.60681 factor:1 | -1 (0.01287) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.45281 HOMO: -6.41644 LUMO: 0.35919 factor:1 | -1 (0.32939) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.54781 HOMO: -6.41917 LUMO: 1.73064 factor:1 | -1 (0.23440) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.41180 HOMO: -4.64226 LUMO: -0.87893 factor:1 | -1 (0.37040) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.63627 HOMO: -6.59604 LUMO: 0.90342 factor:1 | -1 (0.14593) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.59573 HOMO: -6.79468 LUMO: 0.50069 factor:1 | -1 (0.18648) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.73935 HOMO: -7.04503 LUMO: 0.52518 factor:1 | -1 (0.04286) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.16050 HOMO: -6.69400 LUMO: 0.54423 factor:1 | 1 (-0.37829) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.59520 HOMO: -6.51713 LUMO: 0.95240 factor:1 | 1 (-0.81299) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.06536 HOMO: -6.88176 LUMO: 1.79323 factor:1 | 1 (-1.28315) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.45601 HOMO: -6.71849 LUMO: 0.28844 factor:1 | 1 (-0.67381) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.46673 HOMO: -6.94979 LUMO: 0.51974 factor:1 | 1 (-0.68453) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.06792 HOMO: -6.76203 LUMO: 0.94151 factor:1 | 1 (-1.28571) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.76654 HOMO: -6.91169 LUMO: 0.89525 factor:1 | 1 (-1.98434) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.51235 HOMO: -6.83006 LUMO: 0.89253 factor:1 | -1 (0.26986) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.64184 HOMO: -7.08857 LUMO: 0.60409 factor:1 | 1 (-0.85963) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.89940 HOMO: -6.91713 LUMO: 1.76330 factor:1 | 1 (-1.11719) | -1 | -1 |
| G: -6154.41651 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.75738 HOMO: -6.47359 LUMO: 1.56193 factor:1 | 1 (-0.97517) | -1 | -1 |
| G: -6154.41651 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.12359 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-1.34139) | -1 | -1 |
| G: -6154.41651 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.65166 HOMO: -7.03686 LUMO: 1.97283 factor:1 | 1 (-0.86946) | -1 | -1 |
| G: -6154.41651 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.29543 HOMO: -7.00965 LUMO: 1.64629 factor:1 | 1 (-1.51323) | -1 | -1 |
| G: -6154.41651 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.49222 HOMO: -7.06952 LUMO: 1.67622 factor:1 | 1 (-1.71002) | 1 | -1 |
| G: -6154.41651 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.93632 HOMO: -6.80557 LUMO: 1.70615 factor:1 | 1 (-1.15412) | -1 | -1 |
| G: -6154.41651 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.27733 HOMO: -6.80829 LUMO: 1.71704 factor:1 | -1 (0.50488) | -1 | -1 |
| G: -6154.41651 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.30535 HOMO: -7.26544 LUMO: 1.89935 factor:1 | -1 (0.47685) | 1 | -1 |
| G: -6154.41651 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.49376 HOMO: -7.00149 LUMO: 1.47214 factor:1 | -1 (0.28844) | -1 | -1 |
| G: -6154.41651 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.74166 HOMO: -7.03686 LUMO: 1.97283 factor:1 | -1 (0.04054) | -1 | -1 |
| G: -6154.41651 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.45967 HOMO: -7.00965 LUMO: 1.64629 factor:1 | -1 (0.32254) | -1 | -1 |
| G: -6154.41651 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.37950 HOMO: -7.06952 LUMO: 1.67622 factor:1 | -1 (0.40270) | -1 | -1 |
| G: -6154.41651 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.25047 HOMO: -6.80557 LUMO: 1.70615 factor:1 | -1 (0.53174) | -1 | -1 |
| G: -6154.41651 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.40574 HOMO: -6.80829 LUMO: 1.71704 factor:1 | -1 (0.37647) | -1 | -1 |
| G: -6154.41651 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.89937 HOMO: -7.26544 LUMO: 1.89935 factor:1 | 1 (-1.11716) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.63946 HOMO: -7.00149 LUMO: 1.75241 factor:1 | 1 (-1.85726) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.91014 HOMO: -6.91169 LUMO: 2.07079 factor:1 | 1 (-1.12794) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.94982 HOMO: -7.11034 LUMO: 1.76330 factor:1 | 1 (-1.16761) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.40753 HOMO: -6.87360 LUMO: 2.02725 factor:1 | -1 (0.37467) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.53783 HOMO: -7.08584 LUMO: 1.82044 factor:1 | -1 (1.24438) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.89415 HOMO: -6.90625 LUMO: 1.68166 factor:1 | 1 (-0.11195) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.50693 HOMO: -6.71577 LUMO: 1.93201 factor:1 | -1 (0.27527) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.58332 HOMO: -6.99605 LUMO: 2.08439 factor:1 | -1 (0.19889) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.30865 HOMO: -7.02326 LUMO: 1.97010 factor:1 | -1 (0.47356) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.53289 HOMO: -6.99877 LUMO: 2.15514 factor:1 | -1 (0.24931) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.23647 HOMO: -6.75387 LUMO: 1.95106 factor:1 | -1 (2.54573) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.07339 HOMO: -7.10761 LUMO: 2.06262 factor:1 | 1 (-0.29119) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.85646 HOMO: -7.03142 LUMO: 1.91568 factor:1 | 1 (-0.07426) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.43960 HOMO: -6.98788 LUMO: 1.98371 factor:1 | 1 (-0.65740) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.07034 HOMO: -6.94707 LUMO: 1.68438 factor:1 | 1 (-1.28813) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.43569 HOMO: -6.88176 LUMO: 2.20684 factor:1 | 1 (-0.65348) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.21664 HOMO: -6.73210 LUMO: 2.18780 factor:1 | -1 (0.56556) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.24002 HOMO: -6.83822 LUMO: 2.06807 factor:1 | -1 (0.54219) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.85029 HOMO: -6.78924 LUMO: 2.42181 factor:1 | 1 (-0.06808) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.24442 HOMO: -6.94707 LUMO: 1.71704 factor:1 | 1 (-0.46221) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12416.28385 HOMO: -6.85183 LUMO: 1.78779 factor:1 | -1 (2.49836) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.98486 HOMO: -6.98788 LUMO: 1.69799 factor:1 | -1 (0.79735) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.92592 HOMO: -6.79468 LUMO: 2.04358 factor:1 | -1 (0.85629) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.12716 HOMO: -6.90081 LUMO: 1.97283 factor:1 | 1 (-0.34496) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.06368 HOMO: -6.79468 LUMO: 2.00820 factor:1 | 1 (-0.28147) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.59322 HOMO: -7.06408 LUMO: 2.29936 factor:1 | -1 (0.18898) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.75031 HOMO: -6.78924 LUMO: 2.13337 factor:1 | -1 (0.03189) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.86817 HOMO: -6.79468 LUMO: 2.35106 factor:1 | 1 (-0.08596) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.61154 HOMO: -6.82734 LUMO: 2.16603 factor:1 | -1 (0.17067) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.43561 HOMO: -6.79740 LUMO: 2.36739 factor:1 | -1 (0.34659) | -1 | -1 |
| G: -6154.41651 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.47172 HOMO: -7.14027 LUMO: 2.10888 factor:1 | -1 (0.31048) | -1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.64727 HOMO: -6.96067 LUMO: 1.59731 factor:1 | -1 (1.13493) | -1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.04613 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.26392) | -1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.95560 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-0.17339) | -1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.17700 HOMO: -7.02326 LUMO: 1.41227 factor:1 | -1 (0.60521) | -1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.09797 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.31576) | -1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.36108 HOMO: -6.51168 LUMO: 1.72520 factor:1 | -1 (0.42112) | -1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.44691 HOMO: -6.98516 LUMO: 1.92929 factor:1 | -1 (0.33530) | -1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.84754 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.06533) | -1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.81399 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.03178) | -1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.70977 HOMO: -6.82462 LUMO: 1.86670 factor:1 | -1 (0.07244) | -1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.41242 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.63022) | -1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.42337 HOMO: -6.62869 LUMO: 1.69527 factor:1 | -1 (0.35884) | -1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.30758 HOMO: -6.84094 LUMO: 1.27349 factor:1 | -1 (0.47462) | -1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.03727 HOMO: -7.07768 LUMO: 1.27621 factor:1 | -1 (0.74494) | 1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.87095 HOMO: -7.06135 LUMO: 1.55105 factor:1 | -1 (0.91125) | 1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.01298 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.23077) | -1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.01231 HOMO: -7.07224 LUMO: 1.65445 factor:1 | -1 (0.76989) | 1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.18094 HOMO: -6.68584 LUMO: 1.91296 factor:1 | -1 (0.60126) | -1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.34257 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.56036) | 1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.40009 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-0.61789) | -1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.93986 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-1.15765) | -1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.98468 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.20248) | -1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.14836 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.36616) | -1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.95734 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.17513) | -1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.96158 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.17938) | -1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.06177 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-0.27957) | -1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.63756 HOMO: -6.95523 LUMO: 1.80684 factor:1 | -1 (1.14465) | -1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.58234 HOMO: -6.66135 LUMO: 1.72792 factor:1 | -1 (0.19987) | -1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.93402 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.15181) | -1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.87914 HOMO: -7.03959 LUMO: 2.06262 factor:1 | -1 (0.90306) | -1 | -1 |
| G: -6154.41651 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.95584 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.17364) | 1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.79516 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-0.01295) | -1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.50435 HOMO: -6.91169 LUMO: 1.37145 factor:1 | -1 (0.27786) | -1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.12183 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-0.33963) | -1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.34846 HOMO: -7.02326 LUMO: 1.41227 factor:1 | -1 (0.43375) | -1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.86047 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.07826) | -1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.46097 HOMO: -6.51168 LUMO: 1.72520 factor:1 | -1 (0.32123) | -1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.54390 HOMO: -6.98516 LUMO: 1.92929 factor:1 | -1 (1.23831) | -1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.82180 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.03959) | -1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.18991 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.40771) | -1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.94196 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.15976) | -1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.84199 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.05978) | -1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.86655 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.08435) | -1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.73531 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-0.95311) | -1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.41762 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-0.63541) | 1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.93082 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.14862) | 1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.58087 HOMO: -6.94162 LUMO: 1.64629 factor:1 | -1 (0.20134) | -1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.96947 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.18727) | 1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.05260 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.27040) | -1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.15174 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.36953) | 1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.00245 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-0.22025) | -1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.86403 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-0.08182) | -1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.65306 HOMO: -6.98516 LUMO: 1.64629 factor:1 | -1 (0.12915) | -1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.65894 HOMO: -6.80285 LUMO: 1.95106 factor:1 | -1 (0.12327) | -1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.43906 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.65686) | -1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.73399 HOMO: -6.64230 LUMO: 1.90480 factor:1 | -1 (0.04822) | -1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.60743 HOMO: -6.93618 LUMO: 2.19324 factor:1 | -1 (0.17478) | -1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.04612 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-1.26391) | -1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.61954 HOMO: -6.66135 LUMO: 1.72792 factor:1 | -1 (0.16267) | -1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.38692 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.60472) | -1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.33519 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.55299) | -1 | -1 |
| G: -6154.41651 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.80841 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.02620) | 1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.72272 HOMO: -6.96067 LUMO: 1.59731 factor:1 | -1 (0.05948) | -1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.43384 HOMO: -6.91169 LUMO: 1.37145 factor:1 | -1 (0.34836) | -1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.54245 HOMO: -6.94707 LUMO: 1.73064 factor:1 | -1 (0.23976) | -1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.39013 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.60793) | -1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.58460 HOMO: -6.72121 LUMO: 1.43132 factor:1 | -1 (0.19761) | -1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.34045 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.55824) | -1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.71063 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.92843) | -1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.37660 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.59440) | -1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.20442 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.42221) | -1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.40325 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.62105) | -1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.97156 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-1.18936) | -1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.50037 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-0.71816) | -1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.68176 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-0.89955) | -1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.08906 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.30685) | -1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.45860 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.67639) | -1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.99009 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.20789) | -1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.34388 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.56167) | -1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.42087 HOMO: -6.68584 LUMO: 1.91296 factor:1 | -1 (0.36134) | -1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.97428 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.19208) | -1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.53718 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-0.75498) | -1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.09969 HOMO: -6.93618 LUMO: 1.63540 factor:1 | -1 (0.68252) | -1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.55261 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.77041) | -1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.09209 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.30988) | -1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.36595 HOMO: -6.76747 LUMO: 1.88303 factor:1 | -1 (0.41625) | -1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.31794 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.53574) | -1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.91257 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.13036) | -1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.75773 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.97553) | -1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.88769 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-2.10548) | -1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.94038 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.15818) | -1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.01480 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-1.23259) | -1 | -1 |
| G: -6154.41651 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.86707 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.08486) | -1 | -1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.22436 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-0.44216) | 1 | 1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.82591 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.04370) | -1 | -1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.84666 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.06445) | 1 | 1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.26374 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.48153) | -1 | -1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.90719 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.12498) | -1 | -1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.62058 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-1.83837) | 1 | 1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.75425 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.97205) | 1 | 1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.17586 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.39366) | 1 | 1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.50848 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.72627) | 1 | 1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.28684 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.50464) | 1 | 1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.87091 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.08871) | 1 | 1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.09750 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-0.31530) | 1 | 1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.85061 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.06840) | -1 | -1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.53944 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-0.75724) | -1 | -1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.46743 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.68523) | -1 | -1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.83100 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-2.04880) | 1 | 1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.37660 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.59440) | 1 | 1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.93999 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-2.15778) | 1 | 1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.78208 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.99987) | 1 | 1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.26814 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.48593) | 1 | 1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.11703 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-1.33483) | 1 | 1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.33829 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-1.55608) | 1 | 1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.24855 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-1.46634) | 1 | 1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.48407 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.70186) | 1 | 1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.43525 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.65305) | 1 | 1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.63675 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-0.85455) | 1 | 1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.08607 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-1.30386) | 1 | 1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.24640 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-1.46419) | 1 | 1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.64029 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.85808) | -1 | -1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.24050 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.45829) | 1 | 1 |
| G: -6154.41651 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.38094 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.59873) | 1 | 1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.59122 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.80901) | 1 | 1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.48957 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.70736) | -1 | -1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.10400 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.32179) | 1 | 1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.70606 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.92385) | -1 | -1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.87353 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.09132) | -1 | -1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.84372 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-1.06152) | -1 | -1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.52930 HOMO: -6.98516 LUMO: 1.92929 factor:1 | -1 (0.25290) | 1 | 1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.23852 HOMO: -6.92802 LUMO: 2.07895 factor:1 | -1 (0.54368) | 1 | 1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.33861 HOMO: -7.02326 LUMO: 1.86398 factor:1 | -1 (0.44360) | 1 | 1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.51624 HOMO: -6.82462 LUMO: 1.86670 factor:1 | -1 (0.26596) | 1 | 1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.76348 HOMO: -6.83278 LUMO: 1.71160 factor:1 | -1 (0.01872) | 1 | 1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.31261 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-0.53040) | 1 | 1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.52579 HOMO: -6.84094 LUMO: 1.27349 factor:1 | -1 (0.25641) | -1 | -1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.60797 HOMO: -7.07768 LUMO: 1.27621 factor:1 | -1 (0.17423) | -1 | -1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.36767 HOMO: -7.06135 LUMO: 1.55105 factor:1 | -1 (0.41454) | -1 | -1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.40086 HOMO: -6.94162 LUMO: 1.64629 factor:1 | -1 (0.38134) | 1 | 1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.71110 HOMO: -7.07224 LUMO: 1.65445 factor:1 | -1 (0.07110) | 1 | 1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.67736 HOMO: -6.68584 LUMO: 1.91296 factor:1 | -1 (0.10485) | 1 | 1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.43482 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.65261) | 1 | 1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.08803 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-0.30583) | 1 | 1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.89558 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-2.11337) | 1 | 1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.81588 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-1.03368) | 1 | 1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.27081 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.48861) | 1 | 1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.58685 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.80464) | 1 | 1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.28238 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.50017) | 1 | 1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.90226 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-0.12006) | 1 | 1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.67053 HOMO: -6.95523 LUMO: 1.80684 factor:1 | -1 (0.11168) | 1 | 1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.00769 HOMO: -6.66135 LUMO: 1.72792 factor:1 | -1 (0.77452) | 1 | 1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.15955 HOMO: -6.36202 LUMO: 1.89391 factor:1 | -1 (0.62265) | -1 | -1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.62819 HOMO: -7.03959 LUMO: 2.06262 factor:1 | -1 (0.15402) | 1 | 1 |
| G: -6154.41651 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.48647 HOMO: -7.08584 LUMO: 2.01092 factor:1 | -1 (0.29573) | 1 | 1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.87608 HOMO: -7.06135 LUMO: 0.75376 factor:1 | 1 (-0.09388) | 1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.76185 HOMO: -5.10213 LUMO: 0.77825 factor:1 | -1 (0.02035) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.97182 HOMO: -5.84228 LUMO: 0.50341 factor:1 | -1 (0.81038) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.04347 HOMO: -5.39874 LUMO: 0.68028 factor:1 | -1 (0.73873) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.30562 HOMO: -5.16744 LUMO: 1.14832 factor:1 | -1 (0.47658) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.08831 HOMO: -5.80963 LUMO: 0.35647 factor:1 | -1 (0.69389) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.73761 HOMO: -5.02322 LUMO: 1.07213 factor:1 | -1 (0.04460) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.56038 HOMO: -5.80963 LUMO: 0.56328 factor:1 | -1 (0.22183) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.41828 HOMO: -5.45316 LUMO: 0.78369 factor:1 | -1 (0.36393) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.54963 HOMO: -5.25452 LUMO: 0.82178 factor:1 | -1 (0.23258) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.63306 HOMO: -5.21370 LUMO: 1.03947 factor:1 | -1 (0.14915) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.99919 HOMO: -6.04365 LUMO: 0.31837 factor:1 | 1 (-0.21698) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.82221 HOMO: -5.86405 LUMO: 0.55511 factor:1 | 1 (-0.04000) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.57491 HOMO: -5.64908 LUMO: 0.71022 factor:1 | -1 (0.20730) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.47395 HOMO: -5.94297 LUMO: 0.68301 factor:1 | 1 (-0.69174) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.76035 HOMO: -6.01916 LUMO: 0.56328 factor:1 | 1 (-0.97814) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.89186 HOMO: -6.05181 LUMO: 0.35103 factor:1 | 1 (-1.10965) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.05636 HOMO: -6.08447 LUMO: 0.48436 factor:1 | 1 (-0.27415) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.24665 HOMO: -5.86950 LUMO: 0.36735 factor:1 | 1 (-0.46444) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.87926 HOMO: -5.33615 LUMO: 0.65852 factor:1 | 1 (-1.09705) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.45876 HOMO: -5.36064 LUMO: 0.86804 factor:1 | 1 (-0.67656) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.56064 HOMO: -5.74160 LUMO: 0.64491 factor:1 | 1 (-0.77844) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.79347 HOMO: -5.23003 LUMO: 0.66124 factor:1 | 1 (-0.01127) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.14157 HOMO: -5.77698 LUMO: 0.84083 factor:1 | -1 (0.64064) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.06570 HOMO: -5.60555 LUMO: 0.84355 factor:1 | -1 (0.71650) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.02172 HOMO: -7.11578 LUMO: -1.62452 factor:1 | 1 (-0.23951) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.39547 HOMO: -7.23279 LUMO: -1.63813 factor:1 | 1 (-0.61326) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.77112 HOMO: -6.68312 LUMO: -0.88709 factor:1 | 1 (-0.98892) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.09309 HOMO: -6.99333 LUMO: -0.88709 factor:1 | 1 (-1.31088) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.98160 HOMO: -7.40694 LUMO: 0.11973 factor:1 | 1 (-1.19940) | 1 | 1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.56611 HOMO: -6.74026 LUMO: -0.72927 factor:1 | 1 (-0.78391) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.35046 HOMO: -6.67223 LUMO: -0.70750 factor:1 | 1 (-0.56826) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.21644 HOMO: -7.06952 LUMO: -1.40139 factor:1 | 1 (-1.43423) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.97308 HOMO: -7.21374 LUMO: -1.13199 factor:1 | 1 (-2.19087) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.95063 HOMO: -6.54706 LUMO: -1.34424 factor:1 | 1 (-1.16843) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.15963 HOMO: -7.51851 LUMO: -1.05852 factor:1 | 1 (-0.37742) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.16189 HOMO: -7.07224 LUMO: -1.89391 factor:1 | 1 (-0.37968) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.28834 HOMO: -6.65863 LUMO: -0.46804 factor:1 | 1 (-0.50613) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.73839 HOMO: -7.24367 LUMO: 0.29388 factor:1 | -1 (0.04381) | 1 | 1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.77641 HOMO: -7.02326 LUMO: -0.87893 factor:1 | -1 (0.00580) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.51309 HOMO: -6.88176 LUMO: 0.71566 factor:1 | 1 (-1.73089) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.17815 HOMO: -6.46543 LUMO: 1.01498 factor:1 | 1 (-1.39594) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.98756 HOMO: -6.30760 LUMO: 0.17687 factor:1 | 1 (-1.20536) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12420.00277 HOMO: -6.73210 LUMO: -1.06941 factor:1 | 1 (-1.22057) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.40352 HOMO: -6.83550 LUMO: -0.75920 factor:1 | 1 (-0.62132) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.39182 HOMO: -6.94707 LUMO: 0.42178 factor:1 | 1 (-0.60962) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.11742 HOMO: -6.77019 LUMO: -0.38096 factor:1 | 1 (-0.33522) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.33220 HOMO: -7.34163 LUMO: 0.35103 factor:1 | 1 (-0.55000) | 1 | 1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.17699 HOMO: -6.87632 LUMO: -0.87349 factor:1 | 1 (-0.39478) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.49699 HOMO: -7.06952 LUMO: -1.47214 factor:1 | 1 (-0.71479) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.35612 HOMO: -6.58788 LUMO: -0.37824 factor:1 | 1 (-0.57392) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.59300 HOMO: -6.92802 LUMO: -1.24900 factor:1 | -1 (0.18920) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.17802 HOMO: -7.01237 LUMO: -1.31975 factor:1 | 1 (-0.39582) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.91905 HOMO: -6.74842 LUMO: 0.45987 factor:1 | 1 (-0.13685) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.36593 HOMO: -6.53890 LUMO: 0.94424 factor:1 | -1 (0.41628) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.30742 HOMO: -6.52257 LUMO: -0.66940 factor:1 | -1 (0.47478) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.10082 HOMO: -6.56883 LUMO: -1.48302 factor:1 | 1 (-0.31862) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.93747 HOMO: -7.21646 LUMO: 0.13061 factor:1 | 1 (-0.15527) | 1 | 1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12417.97808 HOMO: -6.62597 LUMO: -0.64763 factor:1 | -1 (0.80412) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.75023 HOMO: -7.38789 LUMO: 0.31021 factor:1 | -1 (0.03197) | 1 | 1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.01250 HOMO: -6.74570 LUMO: -0.70750 factor:1 | 1 (-0.23029) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.10910 HOMO: -6.95251 LUMO: -1.25989 factor:1 | 1 (-0.32689) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12419.27919 HOMO: -7.13483 LUMO: -0.76736 factor:1 | 1 (-0.49699) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.69888 HOMO: -6.93618 LUMO: -1.24628 factor:1 | -1 (0.08332) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.83674 HOMO: -7.03686 LUMO: 0.26395 factor:1 | 1 (-0.05453) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.31357 HOMO: -6.52257 LUMO: -0.84355 factor:1 | -1 (0.46863) | -1 | -1 |
| G: -6154.41651 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12418.40484 HOMO: -6.83278 LUMO: -0.49525 factor:1 | -1 (0.37737) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83319 HOMO: -7.18381 LUMO: -1.64629 factor:1 | -1 (1.02592) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90577 HOMO: -6.74842 LUMO: -0.81090 factor:1 | -1 (0.95335) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.81143 HOMO: -7.09401 LUMO: -0.92519 factor:1 | -1 (2.04768) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.76632 HOMO: -7.20285 LUMO: -0.81634 factor:1 | -1 (2.09280) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.79222 HOMO: -6.72665 LUMO: 0.77008 factor:1 | -1 (2.06690) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52764 HOMO: -6.80829 LUMO: 0.86532 factor:1 | -1 (1.33148) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26042 HOMO: -6.20964 LUMO: 0.99866 factor:1 | -1 (1.59870) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79540 HOMO: -6.52801 LUMO: 1.07757 factor:1 | -1 (1.06372) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37977 HOMO: -6.74298 LUMO: -0.67756 factor:1 | -1 (1.47935) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89148 HOMO: -7.43959 LUMO: 0.03265 factor:1 | -1 (0.96764) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89268 HOMO: -6.46815 LUMO: -0.29933 factor:1 | -1 (0.96644) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.73235 HOMO: -6.70489 LUMO: -0.97145 factor:1 | -1 (1.12677) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85232 HOMO: -6.30216 LUMO: -1.39322 factor:1 | -1 (1.00679) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83923 HOMO: -7.01782 LUMO: -1.07485 factor:1 | -1 (1.01988) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.54867 HOMO: -6.93074 LUMO: 0.25851 factor:1 | -1 (1.31045) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84936 HOMO: -7.07224 LUMO: 0.09524 factor:1 | -1 (1.00976) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.63082 HOMO: -6.62325 LUMO: -0.45443 factor:1 | -1 (1.22829) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77570 HOMO: -7.09945 LUMO: -1.20274 factor:1 | -1 (1.08342) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90125 HOMO: -6.56067 LUMO: -1.39322 factor:1 | -1 (0.95787) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91543 HOMO: -6.75387 LUMO: -0.72654 factor:1 | -1 (0.94369) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90963 HOMO: -6.28583 LUMO: -2.35651 factor:1 | -1 (0.94949) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.70187 HOMO: -6.55522 LUMO: -1.33608 factor:1 | -1 (1.15725) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78941 HOMO: -7.19741 LUMO: -0.93607 factor:1 | -1 (1.06971) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56812 HOMO: -6.39740 LUMO: -1.14832 factor:1 | -1 (0.29100) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50893 HOMO: -7.11850 LUMO: -0.97417 factor:1 | -1 (0.35018) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55459 HOMO: -6.57699 LUMO: -1.14016 factor:1 | -1 (0.30452) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59323 HOMO: -6.57699 LUMO: -1.31975 factor:1 | -1 (0.26588) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44588 HOMO: -6.69128 LUMO: -0.76736 factor:1 | -1 (0.41323) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45884 HOMO: -7.25728 LUMO: 0.29660 factor:1 | -1 (0.40028) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18817 HOMO: -6.37019 LUMO: -0.95240 factor:1 | -1 (0.67095) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36762 HOMO: -6.48447 LUMO: -0.55511 factor:1 | -1 (0.49149) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61168 HOMO: -6.37291 LUMO: -0.78641 factor:1 | -1 (0.24743) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.49402 HOMO: -6.65863 LUMO: -0.69933 factor:1 | -1 (0.36510) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35258 HOMO: -6.44638 LUMO: -0.16055 factor:1 | -1 (0.50654) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32752 HOMO: -6.41917 LUMO: -0.20136 factor:1 | -1 (0.53160) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39737 HOMO: -7.33347 LUMO: 0.12789 factor:1 | -1 (0.46175) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41280 HOMO: -6.70489 LUMO: -0.52518 factor:1 | -1 (0.44632) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12716 HOMO: -7.25183 LUMO: 0.32109 factor:1 | -1 (0.73196) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31497 HOMO: -7.29265 LUMO: 0.28028 factor:1 | -1 (0.54415) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90392 HOMO: -6.57155 LUMO: -0.51702 factor:1 | -1 (0.95520) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.67308 HOMO: -7.08040 LUMO: 0.39729 factor:1 | -1 (1.18604) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78808 HOMO: -6.24501 LUMO: -0.44627 factor:1 | -1 (1.07104) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57552 HOMO: -6.73754 LUMO: -0.45443 factor:1 | -1 (0.28360) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68622 HOMO: -6.24501 LUMO: 0.38096 factor:1 | -1 (0.17290) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.38402 HOMO: -6.86815 LUMO: -0.91974 factor:1 | 1 (-0.52491) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30242 HOMO: -7.40150 LUMO: 0.36191 factor:1 | 1 (-0.44330) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69574 HOMO: -6.44094 LUMO: -0.64219 factor:1 | -1 (0.16338) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.32936 HOMO: -6.69944 LUMO: -0.80001 factor:1 | 1 (-0.47024) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31957 HOMO: -6.61509 LUMO: -0.70750 factor:1 | -1 (0.53955) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81588 HOMO: -7.52123 LUMO: 0.06803 factor:1 | -1 (0.04324) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06478 HOMO: -7.34163 LUMO: 0.30477 factor:1 | 1 (-0.20566) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50357 HOMO: -6.68584 LUMO: -0.78641 factor:1 | -1 (0.35554) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.73511 HOMO: -6.53890 LUMO: -0.50885 factor:1 | 1 (-0.87599) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69759 HOMO: -6.75659 LUMO: -0.68845 factor:1 | -1 (0.16153) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50123 HOMO: -7.08857 LUMO: 0.43266 factor:1 | -1 (0.35788) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.63628 HOMO: -6.28583 LUMO: -0.46804 factor:1 | -1 (0.22283) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47897 HOMO: -6.50080 LUMO: -0.24762 factor:1 | -1 (0.38014) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35878 HOMO: -6.45454 LUMO: -0.58504 factor:1 | -1 (0.50034) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65881 HOMO: -7.20558 LUMO: 0.20953 factor:1 | -1 (0.20030) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91561 HOMO: -6.35930 LUMO: -0.20681 factor:1 | 1 (-0.05649) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69462 HOMO: -6.36202 LUMO: -0.14422 factor:1 | -1 (0.16449) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78622 HOMO: -6.20692 LUMO: 1.97827 factor:1 | -1 (0.07290) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99569 HOMO: -6.48719 LUMO: 1.74153 factor:1 | 1 (-0.13657) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.66808 HOMO: -6.84638 LUMO: 1.88575 factor:1 | 1 (-0.80897) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.46773 HOMO: -5.90759 LUMO: 2.00820 factor:1 | 1 (-0.60861) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.50604 HOMO: -6.56339 LUMO: 1.99732 factor:1 | 1 (-0.64692) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81286 HOMO: -6.20692 LUMO: 1.75241 factor:1 | -1 (0.04626) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92938 HOMO: -6.16882 LUMO: 1.94017 factor:1 | 1 (-0.07026) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93414 HOMO: -6.80829 LUMO: 1.78507 factor:1 | 1 (-0.07502) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53280 HOMO: -6.58243 LUMO: 1.78235 factor:1 | -1 (0.32632) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39371 HOMO: -5.85045 LUMO: 1.82316 factor:1 | 1 (-0.53459) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27393 HOMO: -5.93752 LUMO: 1.56465 factor:1 | 1 (-0.41481) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.81885 HOMO: -6.59604 LUMO: -0.53334 factor:1 | -1 (1.04026) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80868 HOMO: -7.06135 LUMO: 0.29660 factor:1 | -1 (1.05044) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74021 HOMO: -6.50352 LUMO: 1.61908 factor:1 | -1 (1.11890) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69852 HOMO: -6.68040 LUMO: -0.60681 factor:1 | -1 (0.16060) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50809 HOMO: -6.93618 LUMO: -1.09662 factor:1 | -1 (0.35103) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79768 HOMO: -6.72121 LUMO: -1.14016 factor:1 | -1 (1.06143) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.81499 HOMO: -7.12394 LUMO: -1.24900 factor:1 | -1 (1.04413) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59473 HOMO: -6.71305 LUMO: -0.71566 factor:1 | -1 (0.26439) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45378 HOMO: -7.09401 LUMO: -0.86532 factor:1 | -1 (0.40534) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58011 HOMO: -7.08584 LUMO: -0.92519 factor:1 | 1 (-0.72099) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79966 HOMO: -7.05591 LUMO: 0.11973 factor:1 | -1 (0.05946) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81185 HOMO: -7.14843 LUMO: -1.58370 factor:1 | -1 (0.04727) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.70999 HOMO: -7.36884 LUMO: -1.97010 factor:1 | 1 (-0.85087) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.97770 HOMO: -6.81373 LUMO: -1.72248 factor:1 | 1 (-1.11858) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59060 HOMO: -6.87360 LUMO: -1.03947 factor:1 | -1 (0.26852) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.97187 HOMO: -7.02870 LUMO: -0.87349 factor:1 | 1 (-1.11276) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.61695 HOMO: -7.16476 LUMO: -1.18097 factor:1 | 1 (-0.75784) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84665 HOMO: -7.51851 LUMO: 0.07891 factor:1 | -1 (0.01246) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24233 HOMO: -7.04231 LUMO: -0.83539 factor:1 | 1 (-0.38322) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.28084 HOMO: -6.83278 LUMO: -0.60137 factor:1 | 1 (-0.42172) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20555 HOMO: -6.89809 LUMO: -1.19186 factor:1 | 1 (-0.34643) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65236 HOMO: -7.16476 LUMO: -0.79185 factor:1 | -1 (0.20675) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.22304 HOMO: -6.97156 LUMO: -1.25444 factor:1 | 1 (-0.36393) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.98698 HOMO: -6.84366 LUMO: -0.88437 factor:1 | 1 (-0.12787) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11711 HOMO: -6.91986 LUMO: -1.12655 factor:1 | 1 (-0.25799) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.16505 HOMO: -6.49536 LUMO: -0.29660 factor:1 | 1 (-0.30594) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.71489 HOMO: -6.74842 LUMO: 0.42450 factor:1 | 1 (-0.85577) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.16415 HOMO: -7.34435 LUMO: 0.32109 factor:1 | 1 (-1.30503) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62066 HOMO: -7.16476 LUMO: 0.28572 factor:1 | -1 (0.23845) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.17994 HOMO: -6.74298 LUMO: -0.43538 factor:1 | 1 (-0.32082) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24489 HOMO: -7.19469 LUMO: -1.61091 factor:1 | 1 (-0.38578) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13295 HOMO: -7.35252 LUMO: -1.78235 factor:1 | 1 (-0.27383) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24233 HOMO: -7.25456 LUMO: -1.66806 factor:1 | 1 (-0.38322) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.11865 HOMO: -7.54844 LUMO: -1.07213 factor:1 | 1 (-1.25953) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.84558 HOMO: -7.21918 LUMO: -1.55377 factor:1 | 1 (-0.98647) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25357 HOMO: -7.01782 LUMO: -1.60547 factor:1 | 1 (-0.39446) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25643 HOMO: -7.21646 LUMO: -1.53472 factor:1 | 1 (-0.39731) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05486 HOMO: -6.73754 LUMO: -1.37417 factor:1 | -1 (0.80426) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13817 HOMO: -6.78924 LUMO: 0.66396 factor:1 | 1 (-0.27905) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03760 HOMO: -6.82734 LUMO: 0.61226 factor:1 | 1 (-0.17848) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.48108 HOMO: -6.74026 LUMO: 0.65579 factor:1 | 1 (-1.62196) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.42903 HOMO: -7.10489 LUMO: -1.30887 factor:1 | 1 (-0.56992) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99322 HOMO: -7.05047 LUMO: 0.42722 factor:1 | -1 (0.86589) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10179 HOMO: -6.61237 LUMO: 1.30887 factor:1 | 1 (-0.24267) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.97976 HOMO: -7.05863 LUMO: 0.59049 factor:1 | 1 (-1.12065) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20321 HOMO: -6.26406 LUMO: 0.78641 factor:1 | 1 (-0.34409) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07561 HOMO: -6.70489 LUMO: 0.67756 factor:1 | 1 (-0.21649) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.09479 HOMO: -6.78652 LUMO: -0.94968 factor:1 | 1 (-1.23567) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56091 HOMO: -6.36202 LUMO: -0.94424 factor:1 | -1 (0.29821) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65808 HOMO: -6.81645 LUMO: -1.09934 factor:1 | -1 (0.20104) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38912 HOMO: -7.07224 LUMO: 0.85988 factor:1 | -1 (0.47000) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48639 HOMO: -7.02326 LUMO: 1.10206 factor:1 | 1 (-0.62728) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12356 HOMO: -6.71305 LUMO: 0.84627 factor:1 | 1 (-0.26444) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41271 HOMO: -7.27360 LUMO: 0.88165 factor:1 | -1 (0.44640) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.59293 HOMO: -6.84911 LUMO: 0.59865 factor:1 | 1 (-0.73381) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08286 HOMO: -6.75114 LUMO: -2.49801 factor:1 | -1 (0.77626) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.51328 HOMO: -6.97156 LUMO: 0.53606 factor:1 | 1 (-0.65416) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60080 HOMO: -6.54434 LUMO: 0.73199 factor:1 | -1 (0.25832) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.87530 HOMO: -6.21236 LUMO: 0.99866 factor:1 | 1 (-1.01618) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39687 HOMO: -6.34025 LUMO: 0.50341 factor:1 | 1 (-0.53775) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22257 HOMO: -6.59876 LUMO: -0.69389 factor:1 | -1 (1.63655) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22681 HOMO: -6.54978 LUMO: -1.00682 factor:1 | -1 (0.63231) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36899 HOMO: -6.82462 LUMO: -0.98777 factor:1 | -1 (0.49013) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14923 HOMO: -6.85455 LUMO: -0.68573 factor:1 | -1 (0.70989) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08909 HOMO: -7.55388 LUMO: -0.03265 factor:1 | -1 (0.77003) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23448 HOMO: -6.77019 LUMO: -0.71838 factor:1 | -1 (0.62464) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62151 HOMO: -6.84911 LUMO: -1.25444 factor:1 | -1 (0.23761) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26126 HOMO: -6.95251 LUMO: -1.03675 factor:1 | -1 (0.59786) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.64109 HOMO: -6.80829 LUMO: -0.77280 factor:1 | 1 (-0.78197) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.09920 HOMO: -6.94162 LUMO: -0.94151 factor:1 | 1 (-0.24009) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65916 HOMO: -6.89809 LUMO: -0.90886 factor:1 | 1 (-0.80004) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94339 HOMO: -6.85183 LUMO: -0.88981 factor:1 | 1 (-0.08427) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15041 HOMO: -6.51985 LUMO: -0.84627 factor:1 | 1 (-0.29130) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33624 HOMO: -6.83278 LUMO: -1.08029 factor:1 | 1 (-0.47712) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.47502 HOMO: -6.91986 LUMO: 0.66396 factor:1 | 1 (-0.61590) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56104 HOMO: -6.94162 LUMO: 0.50885 factor:1 | -1 (0.29807) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72020 HOMO: -6.94435 LUMO: 0.80546 factor:1 | -1 (0.13891) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78156 HOMO: -6.74298 LUMO: -0.81634 factor:1 | -1 (0.07755) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57699 HOMO: -7.04503 LUMO: 1.15921 factor:1 | -1 (0.28213) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38839 HOMO: -6.76475 LUMO: 0.75920 factor:1 | -1 (0.47073) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39329 HOMO: -7.05047 LUMO: 0.68845 factor:1 | -1 (0.46583) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.82047 HOMO: -7.12666 LUMO: 0.60681 factor:1 | 1 (-0.96135) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47685 HOMO: -6.90897 LUMO: -1.22723 factor:1 | -1 (0.38227) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13841 HOMO: -7.10761 LUMO: 0.58232 factor:1 | 1 (-0.27930) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.79826 HOMO: -6.57427 LUMO: 0.71294 factor:1 | 1 (-0.93915) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.98444 HOMO: -6.22597 LUMO: 0.99322 factor:1 | 1 (-1.12533) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.50607 HOMO: -6.83550 LUMO: -0.77825 factor:1 | 1 (-0.64695) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02494 HOMO: -7.14843 LUMO: 0.44627 factor:1 | 1 (-0.16583) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10429 HOMO: -7.08040 LUMO: 0.78913 factor:1 | 1 (-0.24517) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.16081 HOMO: -6.81373 LUMO: -0.93879 factor:1 | 1 (-0.30169) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27447 HOMO: -6.95251 LUMO: 0.22585 factor:1 | 1 (-0.41535) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30965 HOMO: -7.13483 LUMO: -1.25444 factor:1 | -1 (1.54947) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.41328 HOMO: -6.37835 LUMO: -1.54289 factor:1 | 1 (-0.55416) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02000 HOMO: -6.53617 LUMO: -1.43948 factor:1 | -1 (0.83912) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52716 HOMO: -6.38379 LUMO: 0.16055 factor:1 | 1 (-0.66804) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02902 HOMO: -6.53617 LUMO: 0.15783 factor:1 | 1 (-0.16991) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.54305 HOMO: -6.79740 LUMO: -0.17960 factor:1 | -1 (2.31607) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91228 HOMO: -6.26678 LUMO: -0.41361 factor:1 | -1 (1.94684) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68272 HOMO: -6.35658 LUMO: -0.24218 factor:1 | 1 (-0.82361) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79354 HOMO: -6.48175 LUMO: -0.71566 factor:1 | -1 (0.06558) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31045 HOMO: -6.21508 LUMO: -0.40001 factor:1 | -1 (0.54866) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36956 HOMO: -6.51985 LUMO: -0.32654 factor:1 | -1 (0.48956) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38625 HOMO: -6.45182 LUMO: -0.66396 factor:1 | -1 (1.47287) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29485 HOMO: -6.51441 LUMO: -0.65307 factor:1 | 1 (-0.43574) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.43872 HOMO: -6.57971 LUMO: -0.92519 factor:1 | 1 (-0.57960) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56243 HOMO: -6.67223 LUMO: -0.58232 factor:1 | -1 (0.29669) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74015 HOMO: -6.10351 LUMO: -0.45987 factor:1 | -1 (0.11897) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62464 HOMO: -6.13889 LUMO: -0.50341 factor:1 | -1 (0.23448) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26097 HOMO: -6.63141 LUMO: -0.28300 factor:1 | -1 (1.59815) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48463 HOMO: -6.37563 LUMO: -0.22858 factor:1 | -1 (0.37448) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48039 HOMO: -6.37019 LUMO: 0.11429 factor:1 | -1 (0.37873) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75873 HOMO: -6.23957 LUMO: 0.28844 factor:1 | -1 (0.10038) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23889 HOMO: -6.41372 LUMO: -0.53879 factor:1 | -1 (0.62023) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.34235 HOMO: -7.06680 LUMO: 0.32654 factor:1 | -1 (0.51677) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04569 HOMO: -6.50896 LUMO: -0.73743 factor:1 | -1 (0.81343) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.73374 HOMO: -6.42189 LUMO: -0.28572 factor:1 | -1 (2.12537) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.25737 HOMO: -6.79740 LUMO: -0.25851 factor:1 | -1 (1.60174) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45082 HOMO: -6.32393 LUMO: 0.17960 factor:1 | -1 (1.40830) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.54029 HOMO: -6.65046 LUMO: 0.03537 factor:1 | -1 (1.31883) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82952 HOMO: -6.60148 LUMO: 0.07619 factor:1 | -1 (1.02960) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08544 HOMO: -6.57971 LUMO: 0.11429 factor:1 | -1 (0.77367) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.04616 HOMO: -6.88448 LUMO: -1.21907 factor:1 | -1 (1.81296) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20540 HOMO: -6.97700 LUMO: 0.36463 factor:1 | -1 (1.65372) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24671 HOMO: -6.73210 LUMO: -0.84083 factor:1 | -1 (1.61241) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23742 HOMO: -6.21236 LUMO: -0.68845 factor:1 | -1 (0.62170) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.56269 HOMO: -6.35658 LUMO: -0.82995 factor:1 | 1 (-0.70358) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60192 HOMO: -6.75114 LUMO: -0.94424 factor:1 | -1 (0.25720) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.36313 HOMO: -6.74026 LUMO: -1.46125 factor:1 | -1 (2.49599) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43479 HOMO: -7.06952 LUMO: 0.91974 factor:1 | -1 (1.42433) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.00142 HOMO: -7.08857 LUMO: 0.74559 factor:1 | -1 (1.85769) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.66427 HOMO: -6.74298 LUMO: 1.03131 factor:1 | -1 (1.19485) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.40231 HOMO: -6.74842 LUMO: -1.77962 factor:1 | 1 (-0.54319) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47922 HOMO: -6.82462 LUMO: -1.61908 factor:1 | -1 (0.37990) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.50408 HOMO: -7.17020 LUMO: -1.02043 factor:1 | 1 (-0.64496) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71642 HOMO: -6.26406 LUMO: -0.96328 factor:1 | -1 (0.14270) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.66023 HOMO: -6.50896 LUMO: -0.38640 factor:1 | -1 (0.19889) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.37511 HOMO: -7.27632 LUMO: -1.17553 factor:1 | -1 (0.48401) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47870 HOMO: -6.54162 LUMO: -1.36873 factor:1 | -1 (0.38042) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.43870 HOMO: -6.42733 LUMO: -1.15648 factor:1 | -1 (0.42042) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.25854 HOMO: -6.73754 LUMO: -2.58780 factor:1 | -1 (1.60057) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50145 HOMO: -7.20285 LUMO: 0.75103 factor:1 | -1 (0.35767) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.18235 HOMO: -6.98788 LUMO: 0.34831 factor:1 | -1 (1.67677) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70423 HOMO: -6.80013 LUMO: -1.11567 factor:1 | -1 (0.15489) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.20158 HOMO: -6.67767 LUMO: -0.82450 factor:1 | -1 (0.65754) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.03454 HOMO: -6.84911 LUMO: -0.21497 factor:1 | -1 (1.82458) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13179 HOMO: -6.23141 LUMO: 0.21769 factor:1 | -1 (1.72732) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84185 HOMO: -6.68312 LUMO: 0.16327 factor:1 | -1 (1.01727) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21133 HOMO: -7.04503 LUMO: -1.04220 factor:1 | -1 (1.64779) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.31531 HOMO: -6.67495 LUMO: -0.71294 factor:1 | 1 (-1.45619) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.00643 HOMO: -6.70216 LUMO: -0.55239 factor:1 | 1 (-1.14731) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29757 HOMO: -6.60420 LUMO: -0.71294 factor:1 | 1 (-0.43846) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.14532 HOMO: -7.40694 LUMO: 0.11973 factor:1 | 1 (-1.28620) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.90825 HOMO: -6.58788 LUMO: -0.29116 factor:1 | 1 (-1.04913) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30064 HOMO: -6.63686 LUMO: -0.32654 factor:1 | -1 (1.55848) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08240 HOMO: -6.85183 LUMO: -0.95512 factor:1 | -1 (0.77672) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17622 HOMO: -6.82189 LUMO: -0.88165 factor:1 | -1 (0.68290) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03513 HOMO: -6.97428 LUMO: -1.03947 factor:1 | -1 (0.82399) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.85231 HOMO: -6.51441 LUMO: -0.05714 factor:1 | 1 (-0.99319) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.02009 HOMO: -6.61509 LUMO: -0.77008 factor:1 | 1 (-1.16097) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12236 HOMO: -7.36340 LUMO: 0.29116 factor:1 | 1 (-0.26324) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20231 HOMO: -6.64230 LUMO: -0.79185 factor:1 | 1 (-0.34319) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.28105 HOMO: -6.56883 LUMO: -1.03403 factor:1 | 1 (-1.42193) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.67486 HOMO: -6.69400 LUMO: -0.77825 factor:1 | 1 (-0.81574) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.08282 HOMO: -6.37019 LUMO: -0.79185 factor:1 | 1 (-0.22370) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38213 HOMO: -6.49808 LUMO: -0.94424 factor:1 | -1 (0.47699) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.17253 HOMO: -6.91713 LUMO: -0.75376 factor:1 | 1 (-1.31341) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.40182 HOMO: -7.13755 LUMO: 0.41361 factor:1 | 1 (-0.54270) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92546 HOMO: -7.12122 LUMO: 0.39457 factor:1 | 1 (-0.06634) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15452 HOMO: -6.59332 LUMO: -0.57144 factor:1 | 1 (-0.29541) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32553 HOMO: -6.62325 LUMO: -0.66940 factor:1 | -1 (0.53359) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.53766 HOMO: -6.90897 LUMO: -0.08708 factor:1 | 1 (-0.67854) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18438 HOMO: -6.65591 LUMO: -0.81090 factor:1 | -1 (0.67473) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.16040 HOMO: -6.65318 LUMO: -0.94696 factor:1 | 1 (-0.30128) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.40005 HOMO: -6.96067 LUMO: -1.03675 factor:1 | 1 (-0.54094) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55070 HOMO: -6.23141 LUMO: -0.66396 factor:1 | -1 (0.30841) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.77829 HOMO: -6.52529 LUMO: -0.78369 factor:1 | 1 (-0.91917) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93286 HOMO: -6.39468 LUMO: -0.40817 factor:1 | 1 (-0.07374) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30070 HOMO: -6.76203 LUMO: -0.20409 factor:1 | 1 (-0.44159) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.31005 HOMO: -6.96611 LUMO: -0.90342 factor:1 | -1 (1.54906) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26711 HOMO: -6.54706 LUMO: -0.87893 factor:1 | -1 (1.59200) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29242 HOMO: -7.24367 LUMO: -0.97689 factor:1 | -1 (1.56670) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20790 HOMO: -6.61781 LUMO: 1.43404 factor:1 | -1 (1.65121) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24287 HOMO: -6.17971 LUMO: 1.79867 factor:1 | -1 (1.61625) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.06706 HOMO: -5.73344 LUMO: 2.13609 factor:1 | -1 (1.79206) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65471 HOMO: -6.72121 LUMO: 2.06807 factor:1 | -1 (0.20441) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70173 HOMO: -6.91169 LUMO: 2.02997 factor:1 | -1 (0.15739) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56679 HOMO: -7.06408 LUMO: 1.41499 factor:1 | -1 (0.29233) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42578 HOMO: -6.94162 LUMO: -0.90070 factor:1 | -1 (0.43334) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15988 HOMO: -7.09401 LUMO: 0.35103 factor:1 | 1 (-0.30077) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.09997 HOMO: -6.78652 LUMO: 0.91974 factor:1 | 1 (-0.24085) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48609 HOMO: -6.32937 LUMO: -1.89119 factor:1 | 1 (-0.62698) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.53956 HOMO: -7.12666 LUMO: -1.06397 factor:1 | 1 (-0.68045) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06223 HOMO: -6.38107 LUMO: -1.43132 factor:1 | -1 (0.79689) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13649 HOMO: -7.09129 LUMO: 0.08980 factor:1 | -1 (0.72263) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33712 HOMO: -6.31304 LUMO: -0.57960 factor:1 | -1 (0.52200) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24923 HOMO: -6.94435 LUMO: -0.74287 factor:1 | -1 (0.60989) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28477 HOMO: -6.35658 LUMO: -1.53472 factor:1 | -1 (0.57435) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41388 HOMO: -6.39740 LUMO: -1.48846 factor:1 | -1 (0.44523) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46442 HOMO: -7.05319 LUMO: -0.33198 factor:1 | -1 (0.39470) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13486 HOMO: -6.68040 LUMO: -0.09252 factor:1 | -1 (0.72426) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40681 HOMO: -6.35930 LUMO: -0.43266 factor:1 | -1 (0.45231) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14359 HOMO: -6.59604 LUMO: -1.45853 factor:1 | -1 (0.71552) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46768 HOMO: -6.46270 LUMO: -1.49391 factor:1 | -1 (0.39144) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03954 HOMO: -7.05863 LUMO: -1.04764 factor:1 | -1 (0.81958) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25200 HOMO: -7.14027 LUMO: -0.81634 factor:1 | -1 (0.60711) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46178 HOMO: -6.80285 LUMO: -0.74287 factor:1 | -1 (0.39734) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23777 HOMO: -6.53890 LUMO: -1.13471 factor:1 | -1 (0.62134) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.49525 HOMO: -6.49808 LUMO: -1.35513 factor:1 | -1 (0.36387) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.34406 HOMO: -6.75931 LUMO: -1.49663 factor:1 | -1 (0.51506) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18727 HOMO: -6.84638 LUMO: -0.77552 factor:1 | -1 (0.67185) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28207 HOMO: -6.65863 LUMO: -1.34696 factor:1 | -1 (0.57704) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24686 HOMO: -6.25590 LUMO: -2.36467 factor:1 | -1 (0.61226) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47070 HOMO: -7.24911 LUMO: 0.33470 factor:1 | -1 (0.38842) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79128 HOMO: -6.65863 LUMO: -0.75648 factor:1 | -1 (0.06784) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90350 HOMO: -6.31576 LUMO: -0.83267 factor:1 | 1 (-0.04438) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99939 HOMO: -6.64774 LUMO: -0.66124 factor:1 | 1 (-0.14027) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81604 HOMO: -6.75387 LUMO: -1.00138 factor:1 | -1 (0.04308) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.87456 HOMO: -6.52529 LUMO: -0.68301 factor:1 | 1 (-1.01545) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.40500 HOMO: -6.59332 LUMO: -0.68028 factor:1 | 1 (-1.54588) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54521 HOMO: -5.98650 LUMO: 0.31565 factor:1 | -1 (0.31391) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14380 HOMO: -6.59876 LUMO: 0.22585 factor:1 | 1 (-0.28469) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.17959 HOMO: -6.72121 LUMO: 0.10340 factor:1 | 1 (-0.32047) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93278 HOMO: -6.09807 LUMO: 0.20136 factor:1 | 1 (-0.07366) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35383 HOMO: -6.31576 LUMO: 0.06259 factor:1 | -1 (0.50529) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32243 HOMO: -6.35658 LUMO: -0.58232 factor:1 | -1 (0.53669) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53280 HOMO: -6.34842 LUMO: -0.55783 factor:1 | -1 (0.32632) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.05756 HOMO: -6.47359 LUMO: -0.57144 factor:1 | -1 (1.80156) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88541 HOMO: -6.42189 LUMO: -0.09796 factor:1 | -1 (0.97371) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32635 HOMO: -6.35658 LUMO: -0.31293 factor:1 | -1 (0.53277) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24403 HOMO: -7.35524 LUMO: 0.10340 factor:1 | -1 (0.61509) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87997 HOMO: -7.10217 LUMO: 0.36463 factor:1 | -1 (0.97915) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28175 HOMO: -6.43549 LUMO: -0.56872 factor:1 | -1 (0.57737) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11674 HOMO: -6.50080 LUMO: -0.71294 factor:1 | -1 (0.74238) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.04018 HOMO: -6.59060 LUMO: -0.57960 factor:1 | 1 (-0.18106) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.16127 HOMO: -6.78924 LUMO: -0.31565 factor:1 | 1 (-0.30216) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.72077 HOMO: -6.35658 LUMO: 0.07891 factor:1 | 1 (-0.86165) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81819 HOMO: -6.74026 LUMO: -0.87621 factor:1 | -1 (0.04093) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.82965 HOMO: -6.54434 LUMO: 0.81906 factor:1 | -1 (0.02947) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30278 HOMO: -6.66135 LUMO: 1.40955 factor:1 | -1 (0.55634) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24343 HOMO: -6.73754 LUMO: -2.54971 factor:1 | -1 (0.61568) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78306 HOMO: -6.65318 LUMO: 0.69389 factor:1 | -1 (0.07606) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.86010 HOMO: -6.73482 LUMO: 0.62858 factor:1 | 1 (-0.00098) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23312 HOMO: -6.83550 LUMO: 0.68573 factor:1 | -1 (0.62600) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14795 HOMO: -6.83278 LUMO: 0.45987 factor:1 | -1 (0.71117) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.77231 HOMO: -6.78380 LUMO: 0.68301 factor:1 | -1 (0.08680) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.66224 HOMO: -6.90625 LUMO: 1.36601 factor:1 | -1 (0.19687) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18928 HOMO: -6.82734 LUMO: 1.48302 factor:1 | -1 (0.66984) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98846 HOMO: -6.44094 LUMO: -0.94424 factor:1 | -1 (0.87066) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.41554 HOMO: -6.91441 LUMO: 0.28844 factor:1 | 1 (-0.55642) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.12137 HOMO: -6.49808 LUMO: -0.51157 factor:1 | 1 (-1.26225) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.18145 HOMO: -7.09673 LUMO: -0.06259 factor:1 | 1 (-1.32234) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71144 HOMO: -6.77019 LUMO: 0.92247 factor:1 | -1 (0.14768) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17608 HOMO: -6.75931 LUMO: 1.13744 factor:1 | -1 (0.68303) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58991 HOMO: -6.15794 LUMO: 1.12383 factor:1 | 1 (-0.73079) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.07348 HOMO: -6.59604 LUMO: 1.19458 factor:1 | 1 (-1.21436) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12386 HOMO: -7.09401 LUMO: 0.60137 factor:1 | 1 (-0.26474) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86419 HOMO: -6.34025 LUMO: 0.48164 factor:1 | -1 (0.99493) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18444 HOMO: -6.72665 LUMO: -2.47624 factor:1 | -1 (0.67468) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92998 HOMO: -6.48175 LUMO: 0.58232 factor:1 | -1 (0.92913) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.53592 HOMO: -6.94162 LUMO: 0.28300 factor:1 | 1 (-0.67680) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.93919 HOMO: -6.65591 LUMO: 0.57144 factor:1 | 1 (-1.08007) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12407 HOMO: -6.58788 LUMO: -1.03947 factor:1 | 1 (-0.26496) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62643 HOMO: -7.18108 LUMO: 0.37824 factor:1 | -1 (0.23268) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82791 HOMO: -6.63958 LUMO: -1.52112 factor:1 | -1 (1.03120) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06577 HOMO: -6.12528 LUMO: -0.53606 factor:1 | -1 (0.79335) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62962 HOMO: -6.22324 LUMO: -0.87893 factor:1 | -1 (0.22950) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88644 HOMO: -6.62053 LUMO: -0.91974 factor:1 | 1 (-0.02732) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.72240 HOMO: -6.84366 LUMO: -0.83811 factor:1 | 1 (-0.86328) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58506 HOMO: -7.26000 LUMO: 0.25851 factor:1 | 1 (-0.72595) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10503 HOMO: -6.49536 LUMO: -0.63403 factor:1 | 1 (-0.24591) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.55483 HOMO: -6.45726 LUMO: -0.77825 factor:1 | 1 (-0.69571) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.85531 HOMO: -6.74570 LUMO: -0.75103 factor:1 | -1 (0.00381) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88217 HOMO: -7.20285 LUMO: 0.10612 factor:1 | 1 (-0.02305) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18350 HOMO: -6.45182 LUMO: -0.56600 factor:1 | 1 (-0.32439) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32498 HOMO: -6.83278 LUMO: -0.71838 factor:1 | -1 (0.53413) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28673 HOMO: -7.01510 LUMO: -1.09662 factor:1 | -1 (1.57238) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52709 HOMO: -6.48719 LUMO: 0.16871 factor:1 | -1 (1.33202) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.63118 HOMO: -7.30898 LUMO: 0.26667 factor:1 | -1 (2.22793) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89485 HOMO: -6.68856 LUMO: -0.78641 factor:1 | -1 (0.96426) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78612 HOMO: -6.56883 LUMO: -1.00682 factor:1 | -1 (1.07300) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24695 HOMO: -6.41100 LUMO: -0.48980 factor:1 | -1 (1.61217) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45307 HOMO: -6.52257 LUMO: -0.59865 factor:1 | -1 (0.40605) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65634 HOMO: -6.63686 LUMO: -0.56055 factor:1 | -1 (0.20278) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08278 HOMO: -6.79740 LUMO: -0.75376 factor:1 | -1 (0.77634) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96465 HOMO: -5.89127 LUMO: 0.22313 factor:1 | -1 (0.89447) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97159 HOMO: -6.34842 LUMO: 0.11429 factor:1 | -1 (0.88753) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95023 HOMO: -6.13617 LUMO: 1.94834 factor:1 | -1 (0.90889) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.59009 HOMO: -6.50080 LUMO: 1.74153 factor:1 | -1 (1.26903) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.69554 HOMO: -6.33481 LUMO: 1.68438 factor:1 | 1 (-0.83642) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87419 HOMO: -6.53073 LUMO: 1.95106 factor:1 | 1 (-0.01508) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80918 HOMO: -6.46270 LUMO: 1.89935 factor:1 | -1 (0.04993) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71264 HOMO: -5.87222 LUMO: 1.91568 factor:1 | -1 (0.14648) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03058 HOMO: -6.07630 LUMO: 1.81500 factor:1 | 1 (-0.17146) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43988 HOMO: -6.20964 LUMO: 1.81500 factor:1 | -1 (1.41924) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73931 HOMO: -6.15522 LUMO: 1.90752 factor:1 | -1 (0.11981) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48597 HOMO: -6.11984 LUMO: 1.95378 factor:1 | -1 (0.37315) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98628 HOMO: -6.58516 LUMO: 2.04358 factor:1 | -1 (0.87283) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89610 HOMO: -7.37156 LUMO: 0.24490 factor:1 | 1 (-0.03698) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74633 HOMO: -6.36474 LUMO: -0.90070 factor:1 | -1 (0.11279) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99940 HOMO: -6.43549 LUMO: -0.40817 factor:1 | -1 (0.85972) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57248 HOMO: -7.32258 LUMO: 0.29388 factor:1 | -1 (1.28664) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.56516 HOMO: -6.41372 LUMO: -0.20409 factor:1 | -1 (1.29396) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76350 HOMO: -7.18381 LUMO: 0.42722 factor:1 | -1 (0.09562) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67699 HOMO: -6.53890 LUMO: -0.54151 factor:1 | -1 (0.18213) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22275 HOMO: -6.61509 LUMO: 0.08708 factor:1 | -1 (0.63637) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65946 HOMO: -6.78108 LUMO: 2.03541 factor:1 | 1 (-0.80034) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.04738 HOMO: -6.50896 LUMO: 1.53472 factor:1 | 1 (-1.18827) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.16342 HOMO: -6.65591 LUMO: 1.80411 factor:1 | 1 (-0.30430) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.90148 HOMO: -6.64502 LUMO: 1.52112 factor:1 | 1 (-1.04236) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.00176 HOMO: -6.72938 LUMO: 1.48030 factor:1 | 1 (-0.14264) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.17567 HOMO: -6.16882 LUMO: 1.96466 factor:1 | 1 (-0.31655) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91833 HOMO: -6.22597 LUMO: 1.43132 factor:1 | 1 (-0.05921) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42191 HOMO: -6.57699 LUMO: 2.05718 factor:1 | -1 (0.43721) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70951 HOMO: -6.52529 LUMO: 1.89663 factor:1 | -1 (0.14961) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46575 HOMO: -6.30760 LUMO: 1.88031 factor:1 | -1 (0.39337) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39972 HOMO: -6.14977 LUMO: 1.92657 factor:1 | -1 (1.45940) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33942 HOMO: -6.20964 LUMO: 1.83949 factor:1 | -1 (1.51970) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94108 HOMO: -6.31848 LUMO: 1.91296 factor:1 | 1 (-0.08196) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06747 HOMO: -5.80691 LUMO: 2.19868 factor:1 | 1 (-0.20836) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.29334 HOMO: -6.00827 LUMO: 2.15514 factor:1 | -1 (0.56578) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11418 HOMO: -6.51713 LUMO: 2.08711 factor:1 | -1 (0.74494) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.87190 HOMO: -6.32937 LUMO: 2.11705 factor:1 | 1 (-1.01278) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.25231 HOMO: -6.26678 LUMO: 1.95922 factor:1 | 1 (-1.39320) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.74561 HOMO: -6.43005 LUMO: 2.56603 factor:1 | 1 (-0.88649) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.04194 HOMO: -6.41644 LUMO: 2.68304 factor:1 | 1 (-1.18282) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.94232 HOMO: -5.97834 LUMO: 2.02997 factor:1 | 1 (-1.08320) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23186 HOMO: -6.14161 LUMO: 1.77690 factor:1 | 1 (-0.37274) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06327 HOMO: -6.21508 LUMO: 1.80411 factor:1 | -1 (0.79585) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88548 HOMO: -6.46270 LUMO: 2.34562 factor:1 | 1 (-0.02637) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90157 HOMO: -6.39195 LUMO: -0.75920 factor:1 | 1 (-0.04245) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.85052 HOMO: -7.08584 LUMO: -1.14016 factor:1 | -1 (0.00860) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16980 HOMO: -6.70216 LUMO: -0.65035 factor:1 | -1 (0.68932) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.73492 HOMO: -6.79468 LUMO: -0.83811 factor:1 | 1 (-0.87580) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.66286 HOMO: -6.99877 LUMO: -0.79729 factor:1 | 1 (-0.80374) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10824 HOMO: -7.08040 LUMO: -0.85444 factor:1 | 1 (-0.24912) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.86836 HOMO: -7.39333 LUMO: 0.12789 factor:1 | 1 (-1.00924) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13763 HOMO: -7.05047 LUMO: 0.13878 factor:1 | 1 (-0.27851) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14179 HOMO: -6.90897 LUMO: -0.77552 factor:1 | 1 (-0.28267) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.27560 HOMO: -7.25456 LUMO: 0.05170 factor:1 | -1 (1.58351) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.27626 HOMO: -6.84638 LUMO: -0.84355 factor:1 | -1 (1.58286) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95837 HOMO: -6.78108 LUMO: -0.81634 factor:1 | -1 (0.90075) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04563 HOMO: -6.74570 LUMO: -0.77280 factor:1 | -1 (0.81348) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92528 HOMO: -7.28177 LUMO: -1.68438 factor:1 | -1 (0.93384) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04637 HOMO: -7.22190 LUMO: -1.63540 factor:1 | -1 (0.81275) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12026 HOMO: -7.15932 LUMO: -1.57554 factor:1 | -1 (1.73886) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91057 HOMO: -6.57971 LUMO: -0.93063 factor:1 | 1 (-0.05146) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.04592 HOMO: -6.88176 LUMO: 0.58232 factor:1 | 1 (-0.18681) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.80289 HOMO: -6.85727 LUMO: 0.51430 factor:1 | 1 (-0.94377) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33151 HOMO: -6.83550 LUMO: 0.87893 factor:1 | 1 (-0.47239) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96486 HOMO: -7.06680 LUMO: 0.87621 factor:1 | 1 (-0.10574) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19051 HOMO: -6.52257 LUMO: 0.81362 factor:1 | -1 (1.66860) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.05797 HOMO: -6.95523 LUMO: 1.17009 factor:1 | -1 (1.80115) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88272 HOMO: -7.21374 LUMO: 0.97145 factor:1 | -1 (0.97640) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83033 HOMO: -6.81373 LUMO: -1.54561 factor:1 | -1 (0.02879) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59762 HOMO: -6.86543 LUMO: -1.52656 factor:1 | -1 (0.26150) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14974 HOMO: -6.90081 LUMO: -0.78097 factor:1 | -1 (0.70937) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91085 HOMO: -6.64502 LUMO: -0.82723 factor:1 | 1 (-0.05173) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86704 HOMO: -6.65591 LUMO: -0.82178 factor:1 | -1 (0.99207) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00095 HOMO: -6.79468 LUMO: -1.46397 factor:1 | -1 (0.85817) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83235 HOMO: -7.25728 LUMO: 0.73743 factor:1 | -1 (1.02677) | 1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68967 HOMO: -7.00149 LUMO: 1.30070 factor:1 | -1 (0.16945) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95056 HOMO: -7.07768 LUMO: 0.78097 factor:1 | -1 (0.90856) | 1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69740 HOMO: -6.86271 LUMO: 0.86260 factor:1 | -1 (0.16172) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97839 HOMO: -6.94707 LUMO: 0.39729 factor:1 | -1 (0.88072) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94206 HOMO: -6.79740 LUMO: 0.67484 factor:1 | 1 (-0.08294) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72603 HOMO: -6.91986 LUMO: -1.14288 factor:1 | -1 (0.13309) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84323 HOMO: -6.31576 LUMO: 1.01771 factor:1 | -1 (0.01589) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93961 HOMO: -6.81645 LUMO: 0.81362 factor:1 | 1 (-0.08049) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02211 HOMO: -6.92258 LUMO: -0.99594 factor:1 | 1 (-0.16300) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07052 HOMO: -6.81373 LUMO: 0.61770 factor:1 | 1 (-0.21141) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15114 HOMO: -7.18653 LUMO: 1.19186 factor:1 | -1 (1.70798) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07850 HOMO: -7.00693 LUMO: 0.45715 factor:1 | -1 (0.78061) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98552 HOMO: -7.11306 LUMO: 0.53334 factor:1 | -1 (0.87359) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84100 HOMO: -6.63414 LUMO: -1.64357 factor:1 | -1 (1.01811) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58737 HOMO: -6.22052 LUMO: -0.74015 factor:1 | -1 (1.27175) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06767 HOMO: -6.81101 LUMO: -0.50069 factor:1 | -1 (0.79144) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05739 HOMO: -6.71849 LUMO: -0.51974 factor:1 | -1 (0.80173) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04582 HOMO: -6.72121 LUMO: -1.77690 factor:1 | -1 (0.81329) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92707 HOMO: -6.94162 LUMO: -1.78779 factor:1 | -1 (0.93204) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90917 HOMO: -6.91169 LUMO: 0.88981 factor:1 | -1 (0.94995) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.71572 HOMO: -6.97428 LUMO: 0.70750 factor:1 | -1 (1.14340) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91744 HOMO: -6.74842 LUMO: 1.15921 factor:1 | -1 (0.94168) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83841 HOMO: -7.25183 LUMO: -0.99594 factor:1 | -1 (0.02071) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76769 HOMO: -6.43821 LUMO: -1.00410 factor:1 | -1 (0.09143) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84233 HOMO: -6.52257 LUMO: -0.68573 factor:1 | -1 (0.01679) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54853 HOMO: -6.60148 LUMO: -0.52518 factor:1 | -1 (0.31059) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87030 HOMO: -6.07086 LUMO: -1.39594 factor:1 | 1 (-0.01118) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74722 HOMO: -6.78108 LUMO: -1.54833 factor:1 | -1 (0.11189) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68635 HOMO: -6.73482 LUMO: -1.01498 factor:1 | -1 (0.17277) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80924 HOMO: -6.85183 LUMO: 1.06669 factor:1 | -1 (0.04988) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19154 HOMO: -6.98516 LUMO: 1.43948 factor:1 | -1 (0.66758) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32379 HOMO: -6.94162 LUMO: 0.79185 factor:1 | -1 (0.53533) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03741 HOMO: -6.67495 LUMO: -1.06669 factor:1 | -1 (0.82170) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01880 HOMO: -6.88720 LUMO: -1.00682 factor:1 | -1 (0.84031) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06411 HOMO: -6.85999 LUMO: -0.78097 factor:1 | -1 (0.79501) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99815 HOMO: -6.51713 LUMO: -0.89798 factor:1 | -1 (0.86097) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97001 HOMO: -6.63141 LUMO: -0.91430 factor:1 | -1 (0.88910) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72480 HOMO: -6.63414 LUMO: 0.04354 factor:1 | -1 (0.13432) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65484 HOMO: -6.65046 LUMO: -0.73743 factor:1 | -1 (0.20428) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96954 HOMO: -6.73754 LUMO: -0.71838 factor:1 | 1 (-0.11042) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55555 HOMO: -6.65863 LUMO: -0.60137 factor:1 | -1 (0.30357) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68989 HOMO: -6.61509 LUMO: -0.47892 factor:1 | -1 (0.16923) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80943 HOMO: -6.82189 LUMO: -0.64763 factor:1 | -1 (0.04969) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.98316 HOMO: -6.56883 LUMO: -0.51974 factor:1 | 1 (-1.12405) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30895 HOMO: -6.97428 LUMO: -0.95512 factor:1 | 1 (-0.44983) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52269 HOMO: -6.70489 LUMO: -0.04082 factor:1 | 1 (-0.66358) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.98814 HOMO: -6.74026 LUMO: 0.02177 factor:1 | 1 (-1.12903) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.82132 HOMO: -6.50080 LUMO: -0.89525 factor:1 | -1 (0.03780) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.43718 HOMO: -6.46815 LUMO: -0.61226 factor:1 | -1 (0.42194) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57933 HOMO: -6.57971 LUMO: -0.64219 factor:1 | -1 (0.27979) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67517 HOMO: -7.17836 LUMO: 0.37280 factor:1 | -1 (0.18395) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16823 HOMO: -6.67223 LUMO: 0.12245 factor:1 | -1 (1.69089) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15963 HOMO: -6.55250 LUMO: 0.22858 factor:1 | -1 (1.69949) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74018 HOMO: -6.97156 LUMO: -1.12927 factor:1 | -1 (0.11894) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.66499 HOMO: -6.78924 LUMO: -0.84900 factor:1 | -1 (0.19413) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88521 HOMO: -6.65046 LUMO: -0.65307 factor:1 | 1 (-0.02610) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38080 HOMO: -7.41782 LUMO: 0.08980 factor:1 | -1 (0.47832) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33070 HOMO: -6.56339 LUMO: -0.68573 factor:1 | -1 (0.52842) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35263 HOMO: -6.31032 LUMO: -0.31837 factor:1 | -1 (0.50649) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78962 HOMO: -6.72938 LUMO: -0.45987 factor:1 | -1 (0.06950) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.18573 HOMO: -6.59876 LUMO: -1.03131 factor:1 | -1 (1.67339) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21196 HOMO: -7.29265 LUMO: 0.29660 factor:1 | -1 (1.64716) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37697 HOMO: -6.42189 LUMO: -0.51157 factor:1 | -1 (1.48215) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11138 HOMO: -6.27767 LUMO: -0.52790 factor:1 | -1 (0.74774) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76690 HOMO: -6.41644 LUMO: -0.44627 factor:1 | -1 (0.09222) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30251 HOMO: -6.23413 LUMO: -0.52790 factor:1 | -1 (0.55661) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30178 HOMO: -6.63414 LUMO: -0.44082 factor:1 | -1 (1.55733) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30872 HOMO: -7.03142 LUMO: 0.47076 factor:1 | -1 (1.55040) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26336 HOMO: -6.62053 LUMO: -0.14422 factor:1 | -1 (1.59576) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.11650 HOMO: -6.22324 LUMO: 1.96194 factor:1 | -1 (1.74262) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.17032 HOMO: -6.17971 LUMO: 1.71704 factor:1 | -1 (1.68879) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33808 HOMO: -6.70761 LUMO: 1.68711 factor:1 | -1 (1.52103) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88060 HOMO: -6.52801 LUMO: 1.56193 factor:1 | -1 (0.97852) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86212 HOMO: -6.55794 LUMO: 1.52384 factor:1 | -1 (0.99700) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79700 HOMO: -6.47359 LUMO: 1.82316 factor:1 | -1 (1.06211) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37876 HOMO: -6.65863 LUMO: 1.83133 factor:1 | -1 (1.48035) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16809 HOMO: -6.46270 LUMO: 1.90208 factor:1 | -1 (1.69102) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09038 HOMO: -6.41917 LUMO: 2.03269 factor:1 | -1 (1.76874) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.00556 HOMO: -6.48992 LUMO: 1.87486 factor:1 | -1 (1.85356) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45647 HOMO: -6.51985 LUMO: 1.69527 factor:1 | -1 (0.40265) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10231 HOMO: -6.36202 LUMO: 2.05718 factor:1 | 1 (-0.24319) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.06923 HOMO: -5.96474 LUMO: 1.88575 factor:1 | -1 (1.78988) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.89309 HOMO: -6.56339 LUMO: 2.04630 factor:1 | -1 (1.96602) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.66028 HOMO: -6.43277 LUMO: 1.98371 factor:1 | -1 (0.19883) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84772 HOMO: -6.53345 LUMO: 2.06262 factor:1 | -1 (1.01139) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05937 HOMO: -5.81779 LUMO: 2.11432 factor:1 | -1 (0.79974) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.68519 HOMO: -5.91848 LUMO: 1.86942 factor:1 | -1 (1.17393) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78027 HOMO: -6.48447 LUMO: 1.70343 factor:1 | -1 (1.07885) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45406 HOMO: -6.29671 LUMO: -0.89525 factor:1 | -1 (1.40506) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38997 HOMO: -6.63414 LUMO: -0.76192 factor:1 | -1 (1.46914) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.49702 HOMO: -6.56883 LUMO: -0.86260 factor:1 | -1 (1.36209) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43969 HOMO: -6.93074 LUMO: -0.27483 factor:1 | -1 (1.41943) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.50214 HOMO: -6.85999 LUMO: -0.01905 factor:1 | -1 (1.35698) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.59226 HOMO: -6.26406 LUMO: 0.21769 factor:1 | -1 (1.26685) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53915 HOMO: -6.62325 LUMO: 0.31293 factor:1 | -1 (1.31997) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53945 HOMO: -6.59604 LUMO: 0.19592 factor:1 | -1 (1.31967) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.63368 HOMO: -6.43277 LUMO: -0.27756 factor:1 | -1 (1.22544) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62763 HOMO: -6.54978 LUMO: -0.46531 factor:1 | -1 (0.23149) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70271 HOMO: -6.65046 LUMO: -0.15783 factor:1 | -1 (0.15641) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73218 HOMO: -7.28721 LUMO: 0.23946 factor:1 | -1 (0.12694) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54053 HOMO: -6.71849 LUMO: -0.56600 factor:1 | -1 (0.31859) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14370 HOMO: -6.85183 LUMO: -0.84355 factor:1 | -1 (0.71541) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22569 HOMO: -6.53345 LUMO: -0.84627 factor:1 | -1 (0.63343) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12071 HOMO: -6.60148 LUMO: -0.63130 factor:1 | -1 (0.73841) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20355 HOMO: -6.36202 LUMO: -0.60137 factor:1 | -1 (1.65557) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44379 HOMO: -6.28855 LUMO: -0.52790 factor:1 | -1 (0.41533) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60115 HOMO: -7.07224 LUMO: 0.41906 factor:1 | -1 (0.25796) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71193 HOMO: -6.36202 LUMO: -0.24218 factor:1 | -1 (0.14719) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22368 HOMO: -6.43549 LUMO: 0.14150 factor:1 | -1 (0.63544) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78448 HOMO: -6.76747 LUMO: -0.40545 factor:1 | -1 (0.07464) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44453 HOMO: -6.15249 LUMO: -0.51157 factor:1 | -1 (1.41458) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.49335 HOMO: -6.33753 LUMO: -0.02993 factor:1 | -1 (1.36577) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39999 HOMO: -6.49808 LUMO: -0.83811 factor:1 | -1 (1.45913) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.42894 HOMO: -6.64502 LUMO: -0.46259 factor:1 | -1 (1.43018) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.40864 HOMO: -6.34570 LUMO: 0.22041 factor:1 | -1 (1.45048) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19370 HOMO: -6.63414 LUMO: -0.13606 factor:1 | -1 (1.66542) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12243 HOMO: -6.59604 LUMO: -0.79729 factor:1 | -1 (1.73669) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.08643 HOMO: -7.09401 LUMO: 0.31837 factor:1 | -1 (1.77269) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96786 HOMO: -6.48719 LUMO: -0.31021 factor:1 | -1 (0.89125) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06433 HOMO: -7.11306 LUMO: 0.39729 factor:1 | -1 (0.79479) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.54873 HOMO: -6.95251 LUMO: 0.41089 factor:1 | -1 (1.31039) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.75621 HOMO: -6.61509 LUMO: -0.41906 factor:1 | -1 (1.10290) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00822 HOMO: -6.25318 LUMO: -0.47348 factor:1 | -1 (0.85090) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02735 HOMO: -6.77019 LUMO: -0.10340 factor:1 | -1 (0.83177) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00718 HOMO: -6.54706 LUMO: -0.46259 factor:1 | -1 (0.85193) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00778 HOMO: -6.34297 LUMO: -0.50341 factor:1 | -1 (0.85134) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05935 HOMO: -6.20692 LUMO: -0.51974 factor:1 | -1 (0.79977) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.49779 HOMO: -7.03686 LUMO: 0.46804 factor:1 | -1 (1.36133) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.76473 HOMO: -6.47087 LUMO: 0.22585 factor:1 | -1 (1.09439) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.49057 HOMO: -6.41917 LUMO: 0.19320 factor:1 | -1 (1.36854) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43202 HOMO: -6.61237 LUMO: -0.04354 factor:1 | -1 (1.42710) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43768 HOMO: -6.56339 LUMO: 0.36735 factor:1 | -1 (1.42144) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.06463 HOMO: -6.54978 LUMO: 1.12655 factor:1 | -1 (1.79448) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.81481 HOMO: -6.43277 LUMO: 1.17553 factor:1 | -1 (2.04431) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.80771 HOMO: -6.29944 LUMO: 1.40955 factor:1 | -1 (2.05141) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96950 HOMO: -6.74842 LUMO: 0.74015 factor:1 | -1 (0.88962) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08335 HOMO: -6.15522 LUMO: 1.94289 factor:1 | -1 (0.77577) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17535 HOMO: -6.20147 LUMO: 1.40139 factor:1 | -1 (0.68377) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33207 HOMO: -6.41100 LUMO: 1.40139 factor:1 | -1 (1.52705) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.49011 HOMO: -6.74570 LUMO: 1.80956 factor:1 | -1 (1.36900) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.51175 HOMO: -6.60148 LUMO: -1.04764 factor:1 | -1 (1.34737) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99322 HOMO: -6.82734 LUMO: -0.83267 factor:1 | -1 (0.86589) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28586 HOMO: -7.01782 LUMO: -0.32382 factor:1 | -1 (1.57325) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58554 HOMO: -6.54434 LUMO: 0.11157 factor:1 | -1 (1.27357) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01799 HOMO: -6.53617 LUMO: 0.32926 factor:1 | -1 (0.84113) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07127 HOMO: -6.62597 LUMO: -0.60137 factor:1 | -1 (0.78785) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14563 HOMO: -6.60965 LUMO: -0.75376 factor:1 | -1 (0.71348) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05556 HOMO: -6.29399 LUMO: 0.06803 factor:1 | -1 (0.80355) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30395 HOMO: -6.60692 LUMO: -0.47076 factor:1 | -1 (0.55517) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.62168 HOMO: -7.33891 LUMO: 0.39184 factor:1 | -1 (1.23744) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96003 HOMO: -6.60692 LUMO: 1.46125 factor:1 | -1 (0.89909) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01061 HOMO: -6.21780 LUMO: 2.09256 factor:1 | -1 (0.84851) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08098 HOMO: -6.28311 LUMO: 1.80411 factor:1 | -1 (0.77814) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.21965 HOMO: -6.51168 LUMO: 1.84765 factor:1 | -1 (0.63947) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85698 HOMO: -6.66951 LUMO: 2.01636 factor:1 | -1 (1.00214) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10721 HOMO: -6.75387 LUMO: 1.73881 factor:1 | -1 (0.75191) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92321 HOMO: -6.77291 LUMO: 1.89935 factor:1 | -1 (0.93591) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05524 HOMO: -6.36474 LUMO: 1.61091 factor:1 | -1 (0.80388) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15789 HOMO: -6.60420 LUMO: 1.40955 factor:1 | -1 (1.70123) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.94518 HOMO: -6.81645 LUMO: 1.59731 factor:1 | -1 (1.91394) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04824 HOMO: -5.90215 LUMO: 2.12249 factor:1 | -1 (0.81087) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02740 HOMO: -6.26950 LUMO: 1.62996 factor:1 | -1 (0.83172) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04672 HOMO: -6.41100 LUMO: 1.80684 factor:1 | -1 (0.81240) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00337 HOMO: -6.64230 LUMO: 2.23405 factor:1 | -1 (0.85574) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03094 HOMO: -6.66951 LUMO: 2.21501 factor:1 | -1 (0.82818) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03967 HOMO: -6.90897 LUMO: 2.00004 factor:1 | -1 (0.81944) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.73039 HOMO: -6.61781 LUMO: 1.42043 factor:1 | -1 (1.12873) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.66603 HOMO: -6.56611 LUMO: 1.60003 factor:1 | -1 (1.19308) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77752 HOMO: -6.70489 LUMO: 1.78779 factor:1 | -1 (1.08160) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85831 HOMO: -6.46815 LUMO: 1.59459 factor:1 | -1 (1.00081) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91202 HOMO: -6.31304 LUMO: 1.36873 factor:1 | -1 (0.94709) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.72941 HOMO: -6.22597 LUMO: 1.54833 factor:1 | -1 (1.12971) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08182 HOMO: -5.63004 LUMO: 1.96466 factor:1 | -1 (0.77729) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89028 HOMO: -7.02598 LUMO: 1.79323 factor:1 | -1 (0.96883) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22928 HOMO: -6.78924 LUMO: 2.10888 factor:1 | -1 (0.62983) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52930 HOMO: -6.13345 LUMO: 2.07351 factor:1 | -1 (1.32982) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82827 HOMO: -6.46270 LUMO: -0.37552 factor:1 | -1 (1.03085) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12403 HOMO: -6.51985 LUMO: -0.49525 factor:1 | -1 (0.73509) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.61003 HOMO: -6.60965 LUMO: 1.90480 factor:1 | -1 (1.24908) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58375 HOMO: -6.51168 LUMO: 1.92112 factor:1 | -1 (1.27537) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12642 HOMO: -6.71305 LUMO: 1.91024 factor:1 | -1 (0.73269) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35562 HOMO: -6.86815 LUMO: 2.02997 factor:1 | -1 (0.50349) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23274 HOMO: -6.69944 LUMO: 1.95106 factor:1 | -1 (0.62638) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.21165 HOMO: -6.45182 LUMO: 1.66806 factor:1 | -1 (0.64747) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88163 HOMO: -6.44638 LUMO: 2.16058 factor:1 | -1 (0.97749) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00672 HOMO: -6.65591 LUMO: 1.95106 factor:1 | -1 (0.85240) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79153 HOMO: -6.35114 LUMO: 1.42316 factor:1 | -1 (1.06758) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84508 HOMO: -6.48719 LUMO: 1.59187 factor:1 | -1 (1.01403) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09393 HOMO: -7.05591 LUMO: 1.61908 factor:1 | -1 (0.76518) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19750 HOMO: -6.92258 LUMO: 1.87214 factor:1 | -1 (0.66162) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58807 HOMO: -5.85861 LUMO: 2.11705 factor:1 | -1 (1.27104) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09336 HOMO: -6.27767 LUMO: 1.75513 factor:1 | -1 (0.76576) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.68761 HOMO: -6.16882 LUMO: 1.73881 factor:1 | -1 (1.17150) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79880 HOMO: -6.62053 LUMO: 1.39594 factor:1 | -1 (1.06032) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79542 HOMO: -5.46405 LUMO: 1.68166 factor:1 | -1 (1.06369) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.73110 HOMO: -6.39740 LUMO: 1.68711 factor:1 | -1 (1.12802) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05137 HOMO: -6.99333 LUMO: 2.08439 factor:1 | -1 (0.80774) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47876 HOMO: -6.16882 LUMO: 1.71976 factor:1 | -1 (0.38036) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69294 HOMO: -7.19741 LUMO: 2.24766 factor:1 | -1 (0.16618) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84535 HOMO: -6.77291 LUMO: 2.17691 factor:1 | -1 (0.01377) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58589 HOMO: -6.29944 LUMO: 2.16603 factor:1 | -1 (0.27323) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60540 HOMO: -6.10079 LUMO: 1.83949 factor:1 | -1 (0.25372) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.62266 HOMO: -6.63686 LUMO: 2.05990 factor:1 | -1 (1.23646) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.63870 HOMO: -6.91713 LUMO: 1.87486 factor:1 | -1 (0.22041) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59772 HOMO: -6.63958 LUMO: 1.79323 factor:1 | -1 (0.26139) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55383 HOMO: -6.61781 LUMO: 1.70071 factor:1 | -1 (0.30528) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79552 HOMO: -6.20420 LUMO: 1.82861 factor:1 | -1 (0.06359) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.40649 HOMO: -6.47903 LUMO: -2.16875 factor:1 | -1 (1.45263) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.47501 HOMO: -6.53073 LUMO: 2.18235 factor:1 | -1 (1.38411) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98737 HOMO: -7.01782 LUMO: 1.72520 factor:1 | -1 (0.87174) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86498 HOMO: -6.66135 LUMO: -0.75648 factor:1 | -1 (0.99414) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94389 HOMO: -7.56749 LUMO: 0.22585 factor:1 | -1 (0.91523) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.62715 HOMO: -6.45182 LUMO: -0.71294 factor:1 | -1 (1.23197) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85216 HOMO: -6.31032 LUMO: -0.34286 factor:1 | -1 (1.00696) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83869 HOMO: -6.41917 LUMO: 2.04085 factor:1 | -1 (1.02043) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93611 HOMO: -6.61781 LUMO: 1.98915 factor:1 | -1 (0.92301) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.62160 HOMO: -5.86405 LUMO: 1.57282 factor:1 | -1 (1.23752) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04512 HOMO: -6.44094 LUMO: 1.80956 factor:1 | -1 (0.81400) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91153 HOMO: -6.59060 LUMO: 2.08167 factor:1 | -1 (0.94758) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96087 HOMO: -6.20147 LUMO: 1.69799 factor:1 | -1 (0.89825) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87172 HOMO: -6.50352 LUMO: -0.41361 factor:1 | -1 (0.98739) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92000 HOMO: -6.10896 LUMO: -0.55783 factor:1 | -1 (0.93912) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84560 HOMO: -6.74842 LUMO: -0.56872 factor:1 | -1 (1.01352) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.60364 HOMO: -6.59060 LUMO: -0.22041 factor:1 | -1 (1.25548) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.73325 HOMO: -6.22052 LUMO: -0.60137 factor:1 | -1 (1.12587) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52173 HOMO: -6.65863 LUMO: 0.07891 factor:1 | -1 (1.33739) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89953 HOMO: -6.57427 LUMO: 1.71160 factor:1 | 1 (-0.04041) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.63043 HOMO: -5.84773 LUMO: 1.99459 factor:1 | -1 (0.22868) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56167 HOMO: -6.02188 LUMO: 1.91296 factor:1 | -1 (0.29745) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48286 HOMO: -6.17698 LUMO: 2.00004 factor:1 | 1 (-0.62374) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.17120 HOMO: -6.02732 LUMO: 1.90752 factor:1 | 1 (-1.31208) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.30905 HOMO: -6.68584 LUMO: -0.50885 factor:1 | 1 (-1.44993) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37243 HOMO: -6.61781 LUMO: -0.73471 factor:1 | 1 (-0.51332) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.32321 HOMO: -6.66407 LUMO: -0.79729 factor:1 | 1 (-0.46409) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52593 HOMO: -6.56339 LUMO: 0.23130 factor:1 | 1 (-0.66682) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.09813 HOMO: -6.76747 LUMO: 0.08980 factor:1 | 1 (-1.23902) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.96129 HOMO: -6.70489 LUMO: -0.53334 factor:1 | 1 (-1.10217) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.13846 HOMO: -7.28993 LUMO: 0.10885 factor:1 | 1 (-1.27934) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.45589 HOMO: -6.22052 LUMO: 0.51974 factor:1 | 1 (-0.59677) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.12113 HOMO: -6.81645 LUMO: 0.25307 factor:1 | 1 (-1.26201) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.58731 HOMO: -6.80285 LUMO: 0.02721 factor:1 | 1 (-1.72820) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46388 HOMO: -6.51441 LUMO: 0.08163 factor:1 | -1 (1.39524) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45544 HOMO: -6.73482 LUMO: -0.77008 factor:1 | -1 (0.40368) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22528 HOMO: -6.29127 LUMO: -0.44355 factor:1 | -1 (0.63383) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.17193 HOMO: -6.72938 LUMO: -0.64763 factor:1 | 1 (-1.31281) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.49543 HOMO: -6.49264 LUMO: -0.74559 factor:1 | 1 (-0.63631) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.37136 HOMO: -6.67223 LUMO: -0.55239 factor:1 | 1 (-1.51225) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79645 HOMO: -6.33481 LUMO: 0.33198 factor:1 | -1 (0.06267) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.40002 HOMO: -6.76475 LUMO: -0.25307 factor:1 | -1 (1.45910) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.52273 HOMO: -6.65318 LUMO: 0.03810 factor:1 | -1 (0.33639) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50248 HOMO: -6.09263 LUMO: 0.21497 factor:1 | -1 (0.35663) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40896 HOMO: -6.32120 LUMO: -0.85444 factor:1 | -1 (0.45016) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53791 HOMO: -6.57155 LUMO: -0.67484 factor:1 | -1 (0.32120) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92102 HOMO: -6.53345 LUMO: -0.78913 factor:1 | 1 (-0.06191) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50765 HOMO: -7.07768 LUMO: 0.28844 factor:1 | -1 (0.35146) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.31839 HOMO: -6.75114 LUMO: 0.18776 factor:1 | 1 (-0.45927) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.31583 HOMO: -6.77019 LUMO: -0.12245 factor:1 | 1 (-0.45672) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52610 HOMO: -6.43549 LUMO: 0.16327 factor:1 | 1 (-0.66698) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.28930 HOMO: -6.69400 LUMO: -0.16327 factor:1 | 1 (-0.43018) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65620 HOMO: -6.38651 LUMO: -0.61770 factor:1 | -1 (0.20292) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99082 HOMO: -6.34297 LUMO: -0.33198 factor:1 | 1 (-0.13170) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12658 HOMO: -7.51578 LUMO: 0.02177 factor:1 | 1 (-0.26746) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99175 HOMO: -6.47359 LUMO: -0.22585 factor:1 | 1 (-0.13263) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44431 HOMO: -6.68040 LUMO: -0.47076 factor:1 | -1 (0.41481) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58355 HOMO: -6.75659 LUMO: -0.57688 factor:1 | -1 (0.27557) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67383 HOMO: -6.73754 LUMO: -0.61226 factor:1 | -1 (0.18528) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.56475 HOMO: -7.37429 LUMO: 0.31293 factor:1 | -1 (1.29436) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26932 HOMO: -6.23413 LUMO: -0.90886 factor:1 | -1 (1.58980) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83972 HOMO: -6.51985 LUMO: -0.68028 factor:1 | -1 (0.01940) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26192 HOMO: -6.52257 LUMO: -0.77280 factor:1 | -1 (1.59720) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.95792 HOMO: -7.29537 LUMO: 0.31837 factor:1 | 1 (-0.09880) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96358 HOMO: -6.08447 LUMO: 0.25851 factor:1 | 1 (-0.10446) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.29568 HOMO: -6.20964 LUMO: 0.13606 factor:1 | -1 (0.56344) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.43312 HOMO: -6.49808 LUMO: -0.14150 factor:1 | -1 (0.42599) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17391 HOMO: -7.10761 LUMO: 0.28028 factor:1 | -1 (0.68521) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18406 HOMO: -6.60965 LUMO: -0.62858 factor:1 | -1 (0.67506) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13758 HOMO: -6.40012 LUMO: -0.26939 factor:1 | -1 (0.72154) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16479 HOMO: -6.65318 LUMO: -0.73199 factor:1 | -1 (0.69433) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.13188 HOMO: -6.51441 LUMO: -0.44899 factor:1 | 1 (-1.27276) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.35163 HOMO: -6.28583 LUMO: -0.48708 factor:1 | 1 (-1.49252) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.95448 HOMO: -6.96884 LUMO: 0.19864 factor:1 | 1 (-1.09537) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.40231 HOMO: -6.89809 LUMO: 0.34558 factor:1 | 1 (-0.54319) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90943 HOMO: -6.67495 LUMO: -0.15510 factor:1 | 1 (-0.05031) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65658 HOMO: -7.34980 LUMO: 0.19864 factor:1 | -1 (0.20253) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46491 HOMO: -6.71305 LUMO: -0.81634 factor:1 | -1 (1.39420) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48987 HOMO: -6.39468 LUMO: -0.47076 factor:1 | -1 (1.36925) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50251 HOMO: -6.31304 LUMO: 1.39594 factor:1 | -1 (0.35661) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45789 HOMO: -6.57155 LUMO: 1.55105 factor:1 | -1 (0.40123) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37499 HOMO: -6.68312 LUMO: 1.69255 factor:1 | 1 (-0.51587) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93501 HOMO: -6.61509 LUMO: 1.73881 factor:1 | 1 (-0.07589) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.98151 HOMO: -6.17971 LUMO: 1.90208 factor:1 | 1 (-0.12240) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03251 HOMO: -6.53073 LUMO: 1.73337 factor:1 | 1 (-0.17339) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88943 HOMO: -5.91303 LUMO: 1.90480 factor:1 | 1 (-0.03031) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93950 HOMO: -6.42733 LUMO: 1.80139 factor:1 | 1 (-0.08038) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35462 HOMO: -6.78924 LUMO: 2.31569 factor:1 | -1 (0.50450) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36714 HOMO: -6.04093 LUMO: 1.91568 factor:1 | -1 (0.49198) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87041 HOMO: -6.90081 LUMO: 2.36739 factor:1 | 1 (-0.01129) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96310 HOMO: -6.60965 LUMO: 2.18507 factor:1 | -1 (0.89602) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79710 HOMO: -6.75387 LUMO: 2.48712 factor:1 | -1 (0.06201) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36649 HOMO: -6.56883 LUMO: 1.71432 factor:1 | -1 (1.49263) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29909 HOMO: -6.41644 LUMO: 1.72792 factor:1 | -1 (1.56003) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24926 HOMO: -6.92530 LUMO: 2.54426 factor:1 | -1 (1.60985) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.11386 HOMO: -6.41644 LUMO: 2.70209 factor:1 | -1 (1.74526) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65636 HOMO: -6.29671 LUMO: 2.14698 factor:1 | -1 (0.20275) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11158 HOMO: -6.29127 LUMO: 1.87486 factor:1 | 1 (-0.25247) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21375 HOMO: -6.75931 LUMO: 2.78917 factor:1 | -1 (1.64536) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96359 HOMO: -6.40828 LUMO: 1.86942 factor:1 | -1 (0.89553) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71280 HOMO: -6.45726 LUMO: 1.97010 factor:1 | -1 (0.14632) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83849 HOMO: -6.43277 LUMO: 1.22723 factor:1 | -1 (0.02063) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92521 HOMO: -6.63414 LUMO: 1.62452 factor:1 | 1 (-0.06610) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24126 HOMO: -6.54162 LUMO: 2.16058 factor:1 | -1 (0.61786) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.60239 HOMO: -6.40284 LUMO: 1.88575 factor:1 | -1 (1.25673) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29014 HOMO: -6.20964 LUMO: 1.84221 factor:1 | -1 (1.56898) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.68124 HOMO: -6.58516 LUMO: 1.69799 factor:1 | -1 (1.17787) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44622 HOMO: -6.44094 LUMO: 2.05446 factor:1 | -1 (1.41290) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48192 HOMO: -6.61509 LUMO: 2.16058 factor:1 | -1 (1.37720) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11249 HOMO: -6.65591 LUMO: 1.69527 factor:1 | -1 (0.74663) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90008 HOMO: -5.55112 LUMO: 1.80411 factor:1 | -1 (0.95904) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39686 HOMO: -6.68312 LUMO: 2.38100 factor:1 | -1 (1.46226) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99897 HOMO: -6.51168 LUMO: 2.14698 factor:1 | -1 (0.86015) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98465 HOMO: -6.04637 LUMO: 1.48302 factor:1 | -1 (0.87447) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89777 HOMO: -6.81645 LUMO: -0.74287 factor:1 | -1 (0.96135) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95110 HOMO: -6.96884 LUMO: -0.97961 factor:1 | -1 (0.90802) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98846 HOMO: -6.45998 LUMO: 0.09796 factor:1 | -1 (0.87066) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95695 HOMO: -6.44638 LUMO: 0.09524 factor:1 | -1 (0.90217) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.72609 HOMO: -6.16338 LUMO: -0.54151 factor:1 | -1 (1.13303) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83183 HOMO: -6.35930 LUMO: -0.47892 factor:1 | -1 (1.02728) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33337 HOMO: -6.65318 LUMO: -0.00272 factor:1 | -1 (0.52575) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19328 HOMO: -6.50080 LUMO: 0.14694 factor:1 | -1 (0.66584) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.40663 HOMO: -6.60420 LUMO: 0.94968 factor:1 | -1 (1.45249) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15860 HOMO: -6.60148 LUMO: -0.77552 factor:1 | -1 (1.70052) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21857 HOMO: -6.81645 LUMO: -1.05580 factor:1 | -1 (1.64055) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20834 HOMO: -6.57971 LUMO: -0.82178 factor:1 | -1 (1.65078) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.17754 HOMO: -6.09263 LUMO: -0.45171 factor:1 | -1 (1.68158) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.08834 HOMO: -6.74298 LUMO: -0.61770 factor:1 | -1 (1.77078) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32369 HOMO: -6.72393 LUMO: 1.21091 factor:1 | -1 (1.53543) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16401 HOMO: -6.30488 LUMO: 1.70071 factor:1 | -1 (1.69511) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89379 HOMO: -6.38107 LUMO: 1.55649 factor:1 | -1 (0.96532) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99709 HOMO: -6.17154 LUMO: 1.46669 factor:1 | -1 (0.86203) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85186 HOMO: -6.86543 LUMO: 1.98643 factor:1 | -1 (1.00726) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95094 HOMO: -6.69944 LUMO: 1.65173 factor:1 | -1 (0.90818) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.83870 HOMO: -6.77836 LUMO: 2.16331 factor:1 | -1 (2.02042) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.83818 HOMO: -6.42189 LUMO: 2.36467 factor:1 | -1 (2.02094) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22006 HOMO: -7.00965 LUMO: 2.04358 factor:1 | -1 (0.63906) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10108 HOMO: -6.36746 LUMO: 2.13881 factor:1 | 1 (-0.24196) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.21779 HOMO: -6.37835 LUMO: 1.89935 factor:1 | 1 (-0.35867) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.84180 HOMO: -7.03959 LUMO: 1.27349 factor:1 | -1 (2.01732) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.77397 HOMO: -6.67495 LUMO: -0.89253 factor:1 | -1 (0.08514) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91170 HOMO: -6.71849 LUMO: -0.97961 factor:1 | -1 (0.94742) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62646 HOMO: -6.47903 LUMO: 0.01633 factor:1 | -1 (0.23266) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83118 HOMO: -6.38379 LUMO: 0.01088 factor:1 | -1 (1.02794) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87894 HOMO: -6.49536 LUMO: -0.55239 factor:1 | -1 (0.98018) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.64260 HOMO: -6.53345 LUMO: -0.53879 factor:1 | -1 (1.21651) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53651 HOMO: -6.16610 LUMO: 2.15514 factor:1 | -1 (1.32261) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48418 HOMO: -6.35114 LUMO: 1.98643 factor:1 | -1 (1.37494) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57117 HOMO: -6.43277 LUMO: 2.16058 factor:1 | -1 (1.28794) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17500 HOMO: -6.89809 LUMO: 2.20684 factor:1 | -1 (0.68412) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24885 HOMO: -6.54434 LUMO: 1.93473 factor:1 | -1 (0.61027) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57353 HOMO: -6.72938 LUMO: 2.03269 factor:1 | -1 (0.28558) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25187 HOMO: -6.90353 LUMO: 2.19868 factor:1 | -1 (0.60725) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74263 HOMO: -6.41372 LUMO: 2.02453 factor:1 | -1 (1.11648) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.59893 HOMO: -6.46543 LUMO: 1.90752 factor:1 | -1 (1.26019) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.59275 HOMO: -6.55522 LUMO: 2.11977 factor:1 | -1 (1.26636) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90056 HOMO: -6.28855 LUMO: 2.02181 factor:1 | 1 (-0.04144) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.85259 HOMO: -6.45726 LUMO: 1.52112 factor:1 | -1 (0.00653) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50121 HOMO: -6.37291 LUMO: 2.11705 factor:1 | -1 (0.35791) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.20487 HOMO: -6.88448 LUMO: 2.24494 factor:1 | -1 (0.65424) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09989 HOMO: -6.86271 LUMO: 2.41637 factor:1 | -1 (0.75922) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18321 HOMO: -6.69400 LUMO: 2.34562 factor:1 | -1 (0.67590) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12264 HOMO: -6.18243 LUMO: 2.53882 factor:1 | -1 (0.73648) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46306 HOMO: -6.61237 LUMO: 2.54154 factor:1 | -1 (1.39605) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.21772 HOMO: -6.69672 LUMO: 2.16331 factor:1 | -1 (0.64140) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44508 HOMO: -6.33481 LUMO: 2.34018 factor:1 | -1 (1.41404) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.66658 HOMO: -5.99739 LUMO: 2.37283 factor:1 | -1 (1.19254) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34899 HOMO: -6.49808 LUMO: 2.47351 factor:1 | -1 (1.51012) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.51131 HOMO: -6.22052 LUMO: 1.86398 factor:1 | -1 (1.34781) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.50960 HOMO: -6.32665 LUMO: 2.28031 factor:1 | -1 (1.34952) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29759 HOMO: -5.98378 LUMO: 2.16331 factor:1 | -1 (1.56153) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.31865 HOMO: -6.08991 LUMO: 2.30208 factor:1 | -1 (1.54046) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58481 HOMO: -7.07224 LUMO: 1.55105 factor:1 | -1 (1.27431) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00476 HOMO: -6.84638 LUMO: 1.76874 factor:1 | -1 (0.85436) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14425 HOMO: -6.68856 LUMO: 1.47758 factor:1 | -1 (0.71487) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04049 HOMO: -6.69672 LUMO: 1.71976 factor:1 | -1 (0.81863) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48168 HOMO: -6.86543 LUMO: 2.24766 factor:1 | -1 (1.37744) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.60941 HOMO: -7.21646 LUMO: 1.71976 factor:1 | -1 (1.24971) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.64856 HOMO: -6.94162 LUMO: 2.21773 factor:1 | -1 (0.21056) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65577 HOMO: -6.34842 LUMO: 2.04358 factor:1 | -1 (0.20335) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41448 HOMO: -6.53345 LUMO: 1.96738 factor:1 | -1 (0.44463) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97910 HOMO: -6.34842 LUMO: 1.88303 factor:1 | -1 (0.88002) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.59928 HOMO: -6.38651 LUMO: 2.08983 factor:1 | -1 (1.25983) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75019 HOMO: -6.01372 LUMO: 1.43676 factor:1 | -1 (0.10893) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72516 HOMO: -6.30216 LUMO: 1.41771 factor:1 | -1 (0.13396) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69296 HOMO: -6.52801 LUMO: 1.77146 factor:1 | -1 (0.16615) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53726 HOMO: -6.53617 LUMO: 1.72792 factor:1 | -1 (0.32186) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84064 HOMO: -6.56611 LUMO: 2.20412 factor:1 | -1 (0.01848) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65900 HOMO: -6.66679 LUMO: -0.72927 factor:1 | -1 (0.20011) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80399 HOMO: -6.85455 LUMO: -0.85444 factor:1 | -1 (0.05513) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59370 HOMO: -7.21646 LUMO: 0.27211 factor:1 | -1 (0.26542) | 1 | 1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96656 HOMO: -6.57971 LUMO: -0.41361 factor:1 | -1 (0.89256) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13181 HOMO: -7.03142 LUMO: -1.14288 factor:1 | -1 (0.72731) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28335 HOMO: -6.29944 LUMO: 0.06803 factor:1 | -1 (0.57577) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14686 HOMO: -6.47359 LUMO: 0.28028 factor:1 | -1 (0.71226) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45818 HOMO: -6.42189 LUMO: 1.61364 factor:1 | -1 (0.40093) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12920 HOMO: -6.41100 LUMO: 1.80956 factor:1 | -1 (0.72992) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93759 HOMO: -6.83278 LUMO: 1.83949 factor:1 | 1 (-0.07848) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84323 HOMO: -6.78380 LUMO: -0.76192 factor:1 | -1 (0.01589) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84344 HOMO: -6.95795 LUMO: 2.13609 factor:1 | -1 (0.01567) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72733 HOMO: -6.57155 LUMO: 1.89119 factor:1 | -1 (0.13178) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71226 HOMO: -6.65591 LUMO: 1.93745 factor:1 | -1 (0.14686) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48923 HOMO: -6.44638 LUMO: 2.26943 factor:1 | -1 (0.36988) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.66213 HOMO: -5.88038 LUMO: 1.90480 factor:1 | -1 (0.19698) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39693 HOMO: -6.22052 LUMO: 2.17691 factor:1 | -1 (0.46219) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48186 HOMO: -6.04637 LUMO: 2.23950 factor:1 | -1 (0.37726) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65272 HOMO: -6.44366 LUMO: 2.24766 factor:1 | -1 (0.20640) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65824 HOMO: -6.81917 LUMO: 2.08439 factor:1 | -1 (0.20087) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58798 HOMO: -6.48447 LUMO: 2.28576 factor:1 | -1 (0.27113) | -1 | -1 |
| G: -6258.49342 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.77601 HOMO: -6.54434 LUMO: 1.99187 factor:1 | -1 (0.08310) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73014 HOMO: -6.17698 LUMO: -0.65852 factor:1 | -1 (0.12898) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33897 HOMO: -6.08174 LUMO: -0.58504 factor:1 | -1 (0.52015) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08716 HOMO: -6.55250 LUMO: -0.86804 factor:1 | -1 (0.77196) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28224 HOMO: -6.57699 LUMO: -0.89525 factor:1 | -1 (0.57688) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30694 HOMO: -6.63141 LUMO: -1.04220 factor:1 | -1 (0.55217) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.21391 HOMO: -6.69128 LUMO: -0.76736 factor:1 | -1 (0.64521) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16177 HOMO: -6.25318 LUMO: -1.03131 factor:1 | -1 (0.69735) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17600 HOMO: -6.69944 LUMO: 0.01905 factor:1 | -1 (0.68311) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18885 HOMO: -6.28583 LUMO: 0.38368 factor:1 | -1 (0.67027) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89114 HOMO: -6.90081 LUMO: -0.83811 factor:1 | 1 (-0.03203) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.86004 HOMO: -6.78380 LUMO: -0.10068 factor:1 | 1 (-0.00093) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07295 HOMO: -6.30488 LUMO: -0.98505 factor:1 | -1 (0.78616) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15358 HOMO: -6.29671 LUMO: -1.79051 factor:1 | -1 (0.70554) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.65412 HOMO: -6.76747 LUMO: -0.22041 factor:1 | -1 (1.20500) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10887 HOMO: -6.22597 LUMO: -0.94968 factor:1 | -1 (0.75025) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75476 HOMO: -6.73482 LUMO: 0.05987 factor:1 | -1 (0.10436) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.28955 HOMO: -6.28855 LUMO: 0.34831 factor:1 | 1 (-0.43043) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.77078 HOMO: -6.69400 LUMO: 0.25307 factor:1 | 1 (-0.91166) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.77043 HOMO: -6.70216 LUMO: 0.61226 factor:1 | 1 (-0.91131) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.87111 HOMO: -6.70216 LUMO: 0.17415 factor:1 | 1 (-1.01199) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29801 HOMO: -6.70761 LUMO: 0.24762 factor:1 | 1 (-0.43889) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.50041 HOMO: -6.68856 LUMO: -0.84900 factor:1 | 1 (-0.64129) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.91244 HOMO: -6.71033 LUMO: -0.38640 factor:1 | 1 (-1.05333) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.50199 HOMO: -6.24501 LUMO: -0.09252 factor:1 | 1 (-0.64287) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.04134 HOMO: -6.81645 LUMO: -0.07347 factor:1 | 1 (-1.18223) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30005 HOMO: -6.49536 LUMO: 0.09796 factor:1 | 1 (-0.44093) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.79747 HOMO: -6.71033 LUMO: -0.26395 factor:1 | 1 (-0.93836) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.84050 HOMO: -6.70489 LUMO: -0.09252 factor:1 | 1 (-0.98138) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.12725 HOMO: -6.23685 LUMO: 0.39729 factor:1 | 1 (-1.26813) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.90270 HOMO: -6.69400 LUMO: -0.05442 factor:1 | 1 (-1.04358) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23512 HOMO: -6.36202 LUMO: 0.09796 factor:1 | 1 (-0.37601) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.72558 HOMO: -6.54978 LUMO: 0.15510 factor:1 | 1 (-0.86646) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48778 HOMO: -6.77836 LUMO: 0.25851 factor:1 | 1 (-0.62866) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29659 HOMO: -5.70623 LUMO: 0.73471 factor:1 | 1 (-0.43748) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.42117 HOMO: -5.58378 LUMO: 0.89253 factor:1 | 1 (-0.56205) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30571 HOMO: -5.68718 LUMO: 0.87893 factor:1 | 1 (-0.44659) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96056 HOMO: -5.10486 LUMO: 1.11567 factor:1 | 1 (-0.10144) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10065 HOMO: -4.59328 LUMO: 1.27621 factor:1 | 1 (-0.24153) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11431 HOMO: -4.45450 LUMO: 1.82044 factor:1 | 1 (-0.25519) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15066 HOMO: -4.64226 LUMO: 1.70615 factor:1 | 1 (-0.29154) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20723 HOMO: -5.04227 LUMO: 1.04492 factor:1 | 1 (-0.34812) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23654 HOMO: -4.85723 LUMO: 0.93607 factor:1 | 1 (-0.37742) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.00091 HOMO: -4.72934 LUMO: 1.00410 factor:1 | 1 (-1.14179) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.73165 HOMO: -4.56335 LUMO: 1.56738 factor:1 | 1 (-0.87253) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.96580 HOMO: -5.48854 LUMO: 0.33198 factor:1 | 1 (-1.10669) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25042 HOMO: -4.97424 LUMO: 1.33608 factor:1 | 1 (-0.39130) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.34876 HOMO: -4.60145 LUMO: 1.74697 factor:1 | 1 (-0.48964) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92528 HOMO: -5.60010 LUMO: 0.74831 factor:1 | -1 (0.93384) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04046 HOMO: -5.66541 LUMO: 0.66668 factor:1 | -1 (0.81865) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79136 HOMO: -6.50080 LUMO: 0.07075 factor:1 | -1 (0.06776) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87267 HOMO: -5.79603 LUMO: 0.22313 factor:1 | 1 (-0.01355) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15334 HOMO: -4.68036 LUMO: 1.29798 factor:1 | -1 (0.70578) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30003 HOMO: -4.84363 LUMO: 1.34424 factor:1 | -1 (0.55909) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25678 HOMO: -4.62321 LUMO: 1.82861 factor:1 | 1 (-0.39767) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.21970 HOMO: -5.83684 LUMO: 0.82178 factor:1 | 1 (-0.36058) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29034 HOMO: -5.27629 LUMO: 0.57960 factor:1 | 1 (-0.43122) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92988 HOMO: -5.15928 LUMO: -2.96876 factor:1 | -1 (0.92924) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06490 HOMO: -5.08853 LUMO: 0.89253 factor:1 | -1 (0.79422) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86846 HOMO: -6.42461 LUMO: 0.04354 factor:1 | -1 (0.99066) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83781 HOMO: -6.42733 LUMO: -0.00544 factor:1 | -1 (0.02131) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76807 HOMO: -5.87494 LUMO: 0.69933 factor:1 | -1 (0.09105) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90227 HOMO: -5.07492 LUMO: 1.02587 factor:1 | 1 (-0.04316) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02304 HOMO: -4.44362 LUMO: 1.99187 factor:1 | 1 (-0.16392) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79120 HOMO: -5.82052 LUMO: 0.43810 factor:1 | -1 (0.06792) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83381 HOMO: -5.75793 LUMO: 0.76464 factor:1 | -1 (0.02531) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99351 HOMO: -5.09669 LUMO: 0.72382 factor:1 | 1 (-0.13440) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92878 HOMO: -6.75387 LUMO: -2.02453 factor:1 | 1 (-0.06966) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.53137 HOMO: -5.02322 LUMO: 1.14832 factor:1 | 1 (-0.67226) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.86368 HOMO: -5.75521 LUMO: 0.73471 factor:1 | 1 (-1.00456) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.73358 HOMO: -5.89943 LUMO: 0.54967 factor:1 | 1 (-0.87447) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06429 HOMO: -5.80147 LUMO: 0.72382 factor:1 | 1 (-0.20517) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.08701 HOMO: -6.16066 LUMO: 0.39457 factor:1 | 1 (-0.22790) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58389 HOMO: -5.98650 LUMO: 0.76736 factor:1 | 1 (-0.72478) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88110 HOMO: -4.74839 LUMO: 1.88847 factor:1 | 1 (-0.02199) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73476 HOMO: -5.62459 LUMO: 0.26939 factor:1 | -1 (0.12436) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80453 HOMO: -4.88172 LUMO: 1.30070 factor:1 | -1 (0.05459) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60711 HOMO: -5.09397 LUMO: 0.98505 factor:1 | -1 (0.25200) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.35204 HOMO: -6.50080 LUMO: -0.28300 factor:1 | -1 (1.50708) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.27784 HOMO: -5.04227 LUMO: 1.49935 factor:1 | -1 (1.58128) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.56007 HOMO: -5.22731 LUMO: 0.88437 factor:1 | -1 (1.29904) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30390 HOMO: -4.95519 LUMO: 1.25717 factor:1 | -1 (0.55522) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99030 HOMO: -4.61233 LUMO: 1.27621 factor:1 | 1 (-0.13119) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81920 HOMO: -4.70757 LUMO: 1.63813 factor:1 | -1 (0.03992) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45037 HOMO: -4.85179 LUMO: 1.11839 factor:1 | -1 (0.40874) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48303 HOMO: -4.97696 LUMO: 1.00138 factor:1 | -1 (0.37609) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45427 HOMO: -5.64636 LUMO: 0.81090 factor:1 | -1 (1.40484) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45193 HOMO: -4.37831 LUMO: 1.90208 factor:1 | -1 (1.40718) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58043 HOMO: -4.67764 LUMO: 1.54561 factor:1 | -1 (1.27869) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03197 HOMO: -5.87766 LUMO: 0.42994 factor:1 | -1 (0.82714) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14082 HOMO: -6.03821 LUMO: 0.32382 factor:1 | -1 (0.71830) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98449 HOMO: -5.99739 LUMO: 0.69389 factor:1 | -1 (0.87463) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.47262 HOMO: -6.43821 LUMO: 0.15238 factor:1 | -1 (1.38650) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.50034 HOMO: -6.63414 LUMO: -0.07347 factor:1 | -1 (1.35877) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.41215 HOMO: -6.50080 LUMO: 0.10068 factor:1 | -1 (1.44697) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10246 HOMO: -6.49264 LUMO: 0.19592 factor:1 | -1 (1.75666) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.52395 HOMO: -5.83956 LUMO: 0.12517 factor:1 | -1 (0.33516) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33709 HOMO: -6.50896 LUMO: 0.19048 factor:1 | 1 (-0.47797) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.26326 HOMO: -6.56611 LUMO: 0.04898 factor:1 | 1 (-0.40414) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.17261 HOMO: -6.68040 LUMO: -0.08436 factor:1 | -1 (1.68651) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65367 HOMO: -6.73754 LUMO: -0.08708 factor:1 | -1 (0.20545) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65830 HOMO: -6.80285 LUMO: -0.10612 factor:1 | -1 (0.20082) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97205 HOMO: -6.35658 LUMO: 0.02177 factor:1 | -1 (0.88706) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75718 HOMO: -5.74160 LUMO: 0.14694 factor:1 | -1 (0.10193) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07176 HOMO: -4.78376 LUMO: 0.92791 factor:1 | -1 (0.78736) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18104 HOMO: -5.90215 LUMO: 0.36463 factor:1 | -1 (0.67808) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16109 HOMO: -4.99329 LUMO: 0.85988 factor:1 | -1 (0.69803) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16476 HOMO: -4.93887 LUMO: 1.33608 factor:1 | -1 (0.69435) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26278 HOMO: -5.19193 LUMO: 0.50341 factor:1 | -1 (0.59634) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13875 HOMO: -6.64502 LUMO: -1.98643 factor:1 | -1 (0.72037) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04691 HOMO: -5.15384 LUMO: 0.94968 factor:1 | -1 (0.81221) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14016 HOMO: -6.31032 LUMO: 0.08436 factor:1 | -1 (0.71895) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12095 HOMO: -4.88716 LUMO: 0.82995 factor:1 | -1 (0.73816) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05502 HOMO: -5.57017 LUMO: 0.19320 factor:1 | -1 (0.80410) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26006 HOMO: -4.92254 LUMO: 0.93879 factor:1 | -1 (0.59906) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05350 HOMO: -4.77288 LUMO: 1.60003 factor:1 | -1 (0.80562) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08523 HOMO: -4.97696 LUMO: 0.89798 factor:1 | -1 (0.77389) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09777 HOMO: -5.00690 LUMO: 1.14288 factor:1 | -1 (0.76135) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94922 HOMO: -4.88444 LUMO: 1.48574 factor:1 | -1 (0.90989) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82302 HOMO: -5.03955 LUMO: 1.51023 factor:1 | -1 (1.03610) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04746 HOMO: -5.22459 LUMO: 0.99049 factor:1 | -1 (0.81166) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82310 HOMO: -5.29534 LUMO: 0.96056 factor:1 | -1 (1.03602) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14226 HOMO: -5.35520 LUMO: 0.68301 factor:1 | -1 (0.71686) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42232 HOMO: -5.27357 LUMO: 1.18642 factor:1 | -1 (0.43680) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99584 HOMO: -5.79875 LUMO: 0.61770 factor:1 | -1 (0.86328) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99858 HOMO: -7.64640 LUMO: -2.45175 factor:1 | -1 (0.86053) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.69120 HOMO: -7.46953 LUMO: -1.29798 factor:1 | -1 (1.16791) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04898 HOMO: -7.95389 LUMO: -0.37280 factor:1 | -1 (0.81014) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10950 HOMO: -7.23279 LUMO: -1.19186 factor:1 | -1 (0.74962) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25317 HOMO: -7.14299 LUMO: -1.12927 factor:1 | -1 (0.60594) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12248 HOMO: -6.93074 LUMO: 0.31565 factor:1 | -1 (0.73664) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68709 HOMO: -6.63141 LUMO: 0.28028 factor:1 | -1 (0.17203) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67615 HOMO: -7.10489 LUMO: -1.07213 factor:1 | -1 (0.18297) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.95093 HOMO: -7.00693 LUMO: -0.69389 factor:1 | 1 (-0.09181) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.95422 HOMO: -8.50356 LUMO: -1.79595 factor:1 | 1 (-0.09510) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80363 HOMO: -7.79334 LUMO: -2.33746 factor:1 | -1 (0.05548) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94010 HOMO: -7.24367 LUMO: -0.85172 factor:1 | 1 (-0.08098) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53753 HOMO: -7.94028 LUMO: -0.20136 factor:1 | -1 (0.32158) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10596 HOMO: -7.22462 LUMO: 0.84627 factor:1 | -1 (0.75316) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01905 HOMO: -6.54978 LUMO: 0.34831 factor:1 | -1 (0.84007) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.64907 HOMO: -6.86815 LUMO: 0.32109 factor:1 | -1 (0.21004) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71925 HOMO: -7.17564 LUMO: -1.28438 factor:1 | -1 (0.13987) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78200 HOMO: -7.03142 LUMO: -1.12655 factor:1 | -1 (0.07712) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50937 HOMO: -7.39878 LUMO: 0.15783 factor:1 | -1 (0.34975) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87297 HOMO: -7.25728 LUMO: 0.42178 factor:1 | 1 (-0.01385) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.72702 HOMO: -6.86543 LUMO: 0.93879 factor:1 | 1 (-0.86791) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13624 HOMO: -7.09673 LUMO: -0.69661 factor:1 | 1 (-0.27712) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.75655 HOMO: -7.74708 LUMO: 0.01088 factor:1 | 1 (-0.89743) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.00075 HOMO: -6.80557 LUMO: 0.46531 factor:1 | 1 (-0.14164) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.17031 HOMO: -7.29265 LUMO: 1.31975 factor:1 | 1 (-0.31119) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.79415 HOMO: -6.93618 LUMO: 0.29388 factor:1 | 1 (-0.93504) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39894 HOMO: -6.53073 LUMO: 0.71022 factor:1 | 1 (-0.53982) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.78569 HOMO: -6.41917 LUMO: -1.24084 factor:1 | 1 (-0.92657) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48101 HOMO: -6.67495 LUMO: -1.09118 factor:1 | 1 (-0.62189) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.75611 HOMO: -6.97156 LUMO: -0.53606 factor:1 | 1 (-0.89700) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58561 HOMO: -6.85183 LUMO: -0.45715 factor:1 | 1 (-0.72649) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84445 HOMO: -7.12666 LUMO: -0.67484 factor:1 | -1 (0.01467) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.35355 HOMO: -7.49946 LUMO: -0.14694 factor:1 | 1 (-0.49443) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.95860 HOMO: -7.44231 LUMO: 0.58232 factor:1 | 1 (-0.09948) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99852 HOMO: -7.36340 LUMO: -0.68301 factor:1 | 1 (-0.13940) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.40917 HOMO: -6.13073 LUMO: -0.54967 factor:1 | 1 (-0.55005) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.53524 HOMO: -7.81511 LUMO: -0.06531 factor:1 | 1 (-0.67612) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.31306 HOMO: -7.26816 LUMO: -1.02587 factor:1 | 1 (-0.45394) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30677 HOMO: -7.98110 LUMO: -0.17960 factor:1 | 1 (-0.44765) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20693 HOMO: -7.44776 LUMO: -1.00954 factor:1 | 1 (-0.34782) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.60982 HOMO: -7.47769 LUMO: -1.02859 factor:1 | 1 (-0.75071) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13178 HOMO: -6.75659 LUMO: 0.39457 factor:1 | -1 (0.72733) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89694 HOMO: -6.71849 LUMO: 0.36735 factor:1 | 1 (-0.03782) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87207 HOMO: -7.64096 LUMO: -1.43948 factor:1 | 1 (-0.01295) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70935 HOMO: -7.83144 LUMO: -1.36601 factor:1 | -1 (0.14977) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99006 HOMO: -7.19469 LUMO: 0.35103 factor:1 | 1 (-0.13094) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94832 HOMO: -7.03414 LUMO: 0.20409 factor:1 | 1 (-0.08920) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87928 HOMO: -7.22734 LUMO: 0.31293 factor:1 | 1 (-0.02016) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75590 HOMO: -6.93618 LUMO: 0.56055 factor:1 | -1 (0.10321) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.98467 HOMO: -6.94707 LUMO: -0.88709 factor:1 | 1 (-0.12555) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88630 HOMO: -6.86543 LUMO: -0.83267 factor:1 | 1 (-0.02718) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97060 HOMO: -6.82189 LUMO: -1.15376 factor:1 | 1 (-0.11149) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97213 HOMO: -6.65046 LUMO: -0.46531 factor:1 | 1 (-0.11301) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13069 HOMO: -6.52529 LUMO: 0.20953 factor:1 | 1 (-0.27157) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94949 HOMO: -6.80557 LUMO: 0.44355 factor:1 | -1 (0.90962) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88732 HOMO: -6.93074 LUMO: -0.81634 factor:1 | -1 (0.97180) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90658 HOMO: -7.43143 LUMO: -0.45987 factor:1 | -1 (0.95253) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74620 HOMO: -7.07224 LUMO: -0.68028 factor:1 | -1 (1.11292) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11738 HOMO: -6.68040 LUMO: -0.71566 factor:1 | 1 (-0.25826) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.19409 HOMO: -6.26406 LUMO: -1.09934 factor:1 | 1 (-0.33497) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10486 HOMO: -5.94569 LUMO: -0.72110 factor:1 | 1 (-0.24575) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85483 HOMO: -6.12256 LUMO: -0.42178 factor:1 | -1 (1.00429) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91815 HOMO: -6.09807 LUMO: 0.11429 factor:1 | -1 (0.94097) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.72906 HOMO: -7.35252 LUMO: -0.55783 factor:1 | -1 (1.13006) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.72800 HOMO: -7.57837 LUMO: -0.76736 factor:1 | 1 (-0.86889) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.38343 HOMO: -6.16066 LUMO: 0.01905 factor:1 | 1 (-0.52431) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48264 HOMO: -6.13345 LUMO: -0.41906 factor:1 | 1 (-0.62352) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89912 HOMO: -6.10351 LUMO: -0.33742 factor:1 | 1 (-0.04000) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.61325 HOMO: -7.24639 LUMO: -0.51702 factor:1 | 1 (-0.75414) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87384 HOMO: -6.98244 LUMO: -1.82044 factor:1 | 1 (-0.01472) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74733 HOMO: -6.37563 LUMO: -1.67622 factor:1 | -1 (0.11178) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09597 HOMO: -5.79058 LUMO: -2.55243 factor:1 | -1 (0.76314) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98612 HOMO: -6.34025 LUMO: -0.27483 factor:1 | -1 (0.87300) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95616 HOMO: -6.05453 LUMO: -0.51157 factor:1 | -1 (0.90296) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11720 HOMO: -7.53755 LUMO: -0.38912 factor:1 | -1 (0.74192) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04441 HOMO: -7.00421 LUMO: -0.50885 factor:1 | -1 (0.81471) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98501 HOMO: -7.52123 LUMO: -0.37552 factor:1 | -1 (0.87411) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96228 HOMO: -6.70489 LUMO: -1.04764 factor:1 | -1 (0.89683) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95798 HOMO: -7.06408 LUMO: -1.16737 factor:1 | -1 (0.90113) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77390 HOMO: -6.71849 LUMO: -1.02315 factor:1 | -1 (1.08522) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01303 HOMO: -6.16610 LUMO: -0.50885 factor:1 | -1 (0.84608) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99118 HOMO: -6.48447 LUMO: 0.07619 factor:1 | -1 (0.86793) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.72486 HOMO: -7.06135 LUMO: 0.09796 factor:1 | -1 (1.13425) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79600 HOMO: -6.47359 LUMO: 0.22585 factor:1 | -1 (1.06312) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16248 HOMO: -6.10896 LUMO: -0.62314 factor:1 | -1 (0.69664) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05085 HOMO: -6.88176 LUMO: -0.96600 factor:1 | 1 (-0.19173) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58670 HOMO: -6.67495 LUMO: 0.21769 factor:1 | 1 (-0.72758) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.88254 HOMO: -6.84911 LUMO: 0.38368 factor:1 | 1 (-1.02342) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.42392 HOMO: -6.83550 LUMO: 1.29798 factor:1 | 1 (-0.56480) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.31314 HOMO: -6.67495 LUMO: 1.46941 factor:1 | 1 (-0.45402) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65973 HOMO: -6.81917 LUMO: 1.30887 factor:1 | 1 (-0.80061) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68512 HOMO: -6.56611 LUMO: 0.66396 factor:1 | 1 (-0.82600) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68901 HOMO: -6.76203 LUMO: 0.60137 factor:1 | 1 (-0.82989) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.00448 HOMO: -6.55794 LUMO: 0.34286 factor:1 | 1 (-0.14536) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97814 HOMO: -6.83550 LUMO: 0.35919 factor:1 | 1 (-0.11902) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96403 HOMO: -7.17836 LUMO: 0.63130 factor:1 | -1 (0.89509) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91355 HOMO: -6.29944 LUMO: -0.69389 factor:1 | -1 (0.94557) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04811 HOMO: -7.06680 LUMO: -0.95784 factor:1 | -1 (0.81101) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06512 HOMO: -6.84638 LUMO: -0.87076 factor:1 | -1 (0.79400) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83678 HOMO: -6.96339 LUMO: -1.05308 factor:1 | -1 (0.02234) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62485 HOMO: -6.75387 LUMO: -1.04220 factor:1 | -1 (0.23426) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91931 HOMO: -6.71849 LUMO: -0.84355 factor:1 | 1 (-0.06019) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87104 HOMO: -7.16748 LUMO: 0.51702 factor:1 | 1 (-0.01192) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83743 HOMO: -6.92530 LUMO: 0.71566 factor:1 | -1 (0.02169) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89446 HOMO: -7.11034 LUMO: 0.01905 factor:1 | 1 (-0.03535) | 1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90381 HOMO: -6.79468 LUMO: 0.77008 factor:1 | -1 (0.95531) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.64742 HOMO: -6.52801 LUMO: 0.98233 factor:1 | -1 (1.21170) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.75458 HOMO: -6.76475 LUMO: 0.53334 factor:1 | -1 (1.10454) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92993 HOMO: -5.29261 LUMO: 0.57416 factor:1 | -1 (0.92919) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65448 HOMO: -6.57971 LUMO: 0.12789 factor:1 | 1 (-0.79536) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20467 HOMO: -6.99333 LUMO: 0.51430 factor:1 | 1 (-0.34556) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76409 HOMO: -6.41917 LUMO: 0.19048 factor:1 | -1 (0.09502) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.47325 HOMO: -6.16066 LUMO: 1.77146 factor:1 | 1 (-0.61413) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72151 HOMO: -6.90353 LUMO: 1.65717 factor:1 | -1 (0.13761) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05779 HOMO: -5.94569 LUMO: 1.29526 factor:1 | 1 (-0.19867) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.51562 HOMO: -6.60420 LUMO: 1.33880 factor:1 | 1 (-0.65650) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14318 HOMO: -6.23957 LUMO: 0.09524 factor:1 | 1 (-0.28406) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15948 HOMO: -6.80013 LUMO: 1.34696 factor:1 | 1 (-0.30036) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88807 HOMO: -7.53483 LUMO: -1.52384 factor:1 | 1 (-0.02895) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89075 HOMO: -7.62463 LUMO: -1.65717 factor:1 | -1 (0.96837) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53028 HOMO: -7.62463 LUMO: -1.61364 factor:1 | -1 (1.32884) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44627 HOMO: -8.04096 LUMO: -1.66806 factor:1 | -1 (1.41284) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15560 HOMO: -7.18381 LUMO: -1.17553 factor:1 | -1 (1.70351) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33542 HOMO: -7.69538 LUMO: -1.36601 factor:1 | -1 (1.52370) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44355 HOMO: -7.95117 LUMO: -1.48302 factor:1 | -1 (1.41556) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52435 HOMO: -6.98516 LUMO: 0.35919 factor:1 | 1 (-0.66524) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.66604 HOMO: -7.91579 LUMO: -0.32109 factor:1 | 1 (-0.80693) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.00349 HOMO: -6.75659 LUMO: -0.03537 factor:1 | 1 (-1.14437) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37047 HOMO: -7.78518 LUMO: -2.36467 factor:1 | 1 (-0.51136) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.63285 HOMO: -7.96477 LUMO: -2.75651 factor:1 | 1 (-0.77373) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.95051 HOMO: -7.60286 LUMO: -2.35106 factor:1 | 1 (-1.09139) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65374 HOMO: -7.38245 LUMO: -1.21635 factor:1 | 1 (-0.79463) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.90352 HOMO: -7.91579 LUMO: -1.50479 factor:1 | 1 (-1.04440) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.26777 HOMO: -8.07362 LUMO: -0.28028 factor:1 | 1 (-1.40865) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39320 HOMO: -7.38245 LUMO: -1.15921 factor:1 | -1 (0.46591) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47008 HOMO: -7.18653 LUMO: -0.94968 factor:1 | -1 (0.38904) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97289 HOMO: -6.88448 LUMO: 0.38096 factor:1 | 1 (-0.11377) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05621 HOMO: -6.97972 LUMO: 0.43266 factor:1 | 1 (-0.19709) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.49350 HOMO: -6.88992 LUMO: -0.43538 factor:1 | -1 (0.36561) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.36498 HOMO: -7.97021 LUMO: -0.17143 factor:1 | 1 (-0.50586) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.99974 HOMO: -6.92530 LUMO: 0.77280 factor:1 | 1 (-1.14062) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.51437 HOMO: -7.89674 LUMO: -0.09796 factor:1 | 1 (-0.65525) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.95623 HOMO: -7.02870 LUMO: 0.88709 factor:1 | 1 (-1.09711) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62224 HOMO: -6.78380 LUMO: 0.22041 factor:1 | -1 (0.23688) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45437 HOMO: -7.24911 LUMO: -0.82178 factor:1 | -1 (0.40474) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46627 HOMO: -6.77019 LUMO: 0.52790 factor:1 | -1 (0.39285) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74042 HOMO: -8.56070 LUMO: -1.83405 factor:1 | -1 (0.11870) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.26157 HOMO: -7.74164 LUMO: -2.36195 factor:1 | 1 (-0.40246) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18614 HOMO: -7.39878 LUMO: -2.41637 factor:1 | 1 (-0.32703) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.17474 HOMO: -7.61647 LUMO: -2.34018 factor:1 | 1 (-0.31562) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58066 HOMO: -6.93346 LUMO: -0.57688 factor:1 | -1 (0.27845) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31892 HOMO: -6.85183 LUMO: -1.00410 factor:1 | -1 (0.54020) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46289 HOMO: -7.18925 LUMO: -1.12655 factor:1 | -1 (0.39622) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05972 HOMO: -6.85183 LUMO: -1.60275 factor:1 | 1 (-0.20060) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94108 HOMO: -7.51578 LUMO: 0.12517 factor:1 | 1 (-0.08196) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.19684 HOMO: -7.36068 LUMO: 0.05714 factor:1 | 1 (-0.33772) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65122 HOMO: -7.49674 LUMO: 0.18776 factor:1 | -1 (0.20789) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48335 HOMO: -7.09401 LUMO: -1.24900 factor:1 | -1 (0.37576) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27826 HOMO: -7.22462 LUMO: -1.61364 factor:1 | -1 (0.58085) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.01139 HOMO: -7.74436 LUMO: -0.18776 factor:1 | 1 (-0.15227) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79931 HOMO: -7.35252 LUMO: 0.75376 factor:1 | -1 (0.05981) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12465 HOMO: -7.75252 LUMO: 0.00816 factor:1 | 1 (-0.26553) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.29190 HOMO: -7.06680 LUMO: 0.24490 factor:1 | -1 (0.56722) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54137 HOMO: -7.49129 LUMO: 0.14150 factor:1 | -1 (0.31775) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70067 HOMO: -6.90625 LUMO: -1.11295 factor:1 | -1 (0.15845) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72303 HOMO: -6.78380 LUMO: -0.93063 factor:1 | -1 (0.13608) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23194 HOMO: -7.79878 LUMO: 0.30477 factor:1 | 1 (-0.37282) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61699 HOMO: -7.87498 LUMO: 0.61770 factor:1 | -1 (0.24213) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10606 HOMO: -7.23823 LUMO: 0.30205 factor:1 | 1 (-0.24694) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.22174 HOMO: -7.67633 LUMO: 0.13061 factor:1 | 1 (-0.36262) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65519 HOMO: -7.79606 LUMO: 0.34558 factor:1 | -1 (0.20392) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65386 HOMO: -6.66135 LUMO: -2.60141 factor:1 | -1 (0.20526) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74317 HOMO: -7.03142 LUMO: 0.50885 factor:1 | -1 (0.11595) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.26386 HOMO: -7.05591 LUMO: -0.06531 factor:1 | 1 (-0.40474) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.22043 HOMO: -7.45592 LUMO: -1.39594 factor:1 | 1 (-0.36131) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33443 HOMO: -7.22462 LUMO: -1.10478 factor:1 | -1 (0.52469) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48512 HOMO: -8.14709 LUMO: -0.55783 factor:1 | -1 (0.37399) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54994 HOMO: -7.22190 LUMO: -1.14560 factor:1 | -1 (0.30918) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24715 HOMO: -7.28721 LUMO: -1.14016 factor:1 | 1 (-0.38803) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07654 HOMO: -6.97156 LUMO: 0.51702 factor:1 | 1 (-0.21742) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92540 HOMO: -7.37156 LUMO: 0.29388 factor:1 | 1 (-0.06629) | 1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67819 HOMO: -7.66273 LUMO: -1.59731 factor:1 | -1 (0.18093) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02285 HOMO: -7.50490 LUMO: -1.49935 factor:1 | 1 (-0.16373) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11256 HOMO: -7.61102 LUMO: -1.45581 factor:1 | 1 (-0.25345) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.64286 HOMO: -7.58653 LUMO: -1.61091 factor:1 | 1 (-0.78374) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.62762 HOMO: -7.36068 LUMO: -1.14560 factor:1 | 1 (-0.76850) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05558 HOMO: -6.96339 LUMO: 0.26939 factor:1 | 1 (-0.19647) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07869 HOMO: -6.53617 LUMO: 0.22313 factor:1 | 1 (-0.21957) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52033 HOMO: -7.33619 LUMO: -1.02587 factor:1 | 1 (-0.66121) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.19005 HOMO: -6.87904 LUMO: 0.33742 factor:1 | 1 (-1.33094) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48707 HOMO: -6.88448 LUMO: 0.58777 factor:1 | 1 (-0.62796) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.56308 HOMO: -6.55522 LUMO: -1.51295 factor:1 | 1 (-0.70396) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.17185 HOMO: -7.43415 LUMO: 0.10612 factor:1 | 1 (-1.31273) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.04918 HOMO: -7.54300 LUMO: -0.02449 factor:1 | 1 (-1.19006) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55900 HOMO: -7.42054 LUMO: 0.28028 factor:1 | -1 (0.30011) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13197 HOMO: -6.98244 LUMO: -0.95784 factor:1 | 1 (-0.27285) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10470 HOMO: -6.96884 LUMO: -1.12383 factor:1 | 1 (-0.24558) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06100 HOMO: -6.80829 LUMO: -0.98233 factor:1 | 1 (-0.20188) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50991 HOMO: -7.60830 LUMO: 0.58504 factor:1 | -1 (0.34920) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07139 HOMO: -7.52123 LUMO: 0.08163 factor:1 | 1 (-0.21228) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54172 HOMO: -7.59742 LUMO: 0.00272 factor:1 | -1 (0.31739) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.04960 HOMO: -6.99333 LUMO: -1.33880 factor:1 | 1 (-0.19048) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.86369 HOMO: -6.63958 LUMO: -1.39322 factor:1 | 1 (-0.00457) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11648 HOMO: -7.86137 LUMO: 0.01633 factor:1 | 1 (-0.25737) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45508 HOMO: -7.29537 LUMO: 0.14694 factor:1 | -1 (0.40403) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.08380 HOMO: -6.95523 LUMO: 0.48708 factor:1 | 1 (-0.22468) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02679 HOMO: -7.10217 LUMO: -1.10478 factor:1 | 1 (-0.16768) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92627 HOMO: -6.88176 LUMO: -0.96328 factor:1 | 1 (-0.06716) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47625 HOMO: -7.89130 LUMO: -0.13334 factor:1 | -1 (0.38286) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35143 HOMO: -7.75252 LUMO: 0.25579 factor:1 | -1 (0.50768) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.21042 HOMO: -6.87632 LUMO: -0.93063 factor:1 | 1 (-0.35130) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.57801 HOMO: -6.78108 LUMO: -0.86804 factor:1 | 1 (-0.71890) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.37974 HOMO: -5.98106 LUMO: 0.10340 factor:1 | 1 (-1.52063) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.37958 HOMO: -6.40284 LUMO: -0.87349 factor:1 | 1 (-1.52046) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.38793 HOMO: -6.77019 LUMO: -1.20819 factor:1 | 1 (-1.52882) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06073 HOMO: -6.90081 LUMO: -1.00682 factor:1 | 1 (-0.20161) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99844 HOMO: -6.59060 LUMO: -0.26667 factor:1 | 1 (-0.13932) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65506 HOMO: -6.50896 LUMO: -0.48708 factor:1 | -1 (0.20406) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44858 HOMO: -6.20420 LUMO: -0.73471 factor:1 | -1 (0.41054) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17725 HOMO: -6.17154 LUMO: -0.68573 factor:1 | -1 (0.68186) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06894 HOMO: -6.21236 LUMO: 0.09796 factor:1 | 1 (-0.20983) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.99446 HOMO: -6.38379 LUMO: 0.58232 factor:1 | 1 (-1.13534) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.04992 HOMO: -7.42871 LUMO: 0.40273 factor:1 | 1 (-0.19081) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.06962 HOMO: -6.54978 LUMO: 0.26395 factor:1 | 1 (-1.21050) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.98480 HOMO: -7.14027 LUMO: 0.14150 factor:1 | 1 (-1.12568) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.42789 HOMO: -7.25456 LUMO: -0.15783 factor:1 | 1 (-0.56877) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68814 HOMO: -6.90897 LUMO: 0.63403 factor:1 | 1 (-0.82902) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.34713 HOMO: -6.49264 LUMO: 0.71022 factor:1 | 1 (-0.48801) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.42472 HOMO: -6.56067 LUMO: -1.03947 factor:1 | -1 (1.43439) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03771 HOMO: -6.79196 LUMO: -1.12655 factor:1 | 1 (-0.17859) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13088 HOMO: -6.95251 LUMO: -1.09118 factor:1 | 1 (-0.27176) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81523 HOMO: -7.47225 LUMO: -0.22041 factor:1 | -1 (0.04389) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32801 HOMO: -7.13483 LUMO: -0.98505 factor:1 | -1 (1.53110) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29926 HOMO: -6.99061 LUMO: -1.05852 factor:1 | 1 (-0.44014) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39894 HOMO: -6.52257 LUMO: -1.11022 factor:1 | 1 (-0.53982) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07025 HOMO: -6.75114 LUMO: -1.09934 factor:1 | 1 (-0.21113) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94582 HOMO: -6.82189 LUMO: -0.89253 factor:1 | -1 (0.91330) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06520 HOMO: -6.83278 LUMO: -0.97961 factor:1 | -1 (0.79392) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74008 HOMO: -6.65318 LUMO: -0.84355 factor:1 | -1 (1.11904) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30678 HOMO: -6.75931 LUMO: -0.88437 factor:1 | -1 (0.55234) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.67126 HOMO: -6.19059 LUMO: -0.45715 factor:1 | -1 (1.18786) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.35280 HOMO: -7.09673 LUMO: -2.01908 factor:1 | -1 (1.50631) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05504 HOMO: -7.88042 LUMO: 0.38640 factor:1 | 1 (-0.19592) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.61053 HOMO: -7.83144 LUMO: 0.14422 factor:1 | 1 (-0.75142) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10748 HOMO: -7.46408 LUMO: 0.44627 factor:1 | 1 (-0.24836) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76423 HOMO: -7.12394 LUMO: -2.04902 factor:1 | -1 (0.09489) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55330 HOMO: -6.78380 LUMO: -1.11295 factor:1 | -1 (1.30582) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.49230 HOMO: -7.12938 LUMO: -0.23674 factor:1 | 1 (-0.63318) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65282 HOMO: -6.14705 LUMO: -0.20409 factor:1 | 1 (-0.79370) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24244 HOMO: -6.50080 LUMO: -0.28300 factor:1 | 1 (-0.38333) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15268 HOMO: -6.50352 LUMO: -0.62042 factor:1 | -1 (0.70643) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35293 HOMO: -6.46543 LUMO: -0.53879 factor:1 | -1 (0.50619) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98397 HOMO: -7.32803 LUMO: -0.52790 factor:1 | -1 (0.87515) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68306 HOMO: -5.94025 LUMO: -0.17687 factor:1 | -1 (0.17606) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25768 HOMO: -5.62187 LUMO: 0.05714 factor:1 | 1 (-0.39857) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.45499 HOMO: -7.03414 LUMO: -1.04492 factor:1 | 1 (-0.59587) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.08448 HOMO: -6.75387 LUMO: -2.02181 factor:1 | 1 (-0.22536) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16880 HOMO: -6.55250 LUMO: -0.75648 factor:1 | -1 (1.69032) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.62416 HOMO: -6.81101 LUMO: -1.02043 factor:1 | -1 (1.23496) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45003 HOMO: -6.69672 LUMO: -2.81910 factor:1 | -1 (1.40909) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.85411 HOMO: -6.69128 LUMO: -2.58236 factor:1 | -1 (0.00501) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07681 HOMO: -6.73482 LUMO: -2.06807 factor:1 | 1 (-0.21769) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81631 HOMO: -7.66545 LUMO: 0.17143 factor:1 | -1 (0.04280) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.03663 HOMO: -6.87904 LUMO: -1.25172 factor:1 | -1 (1.82248) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19500 HOMO: -6.84366 LUMO: -0.19320 factor:1 | -1 (1.66411) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11238 HOMO: -6.97972 LUMO: -0.97961 factor:1 | -1 (0.74673) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.29979 HOMO: -6.72121 LUMO: -0.70477 factor:1 | -1 (0.55933) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93028 HOMO: -7.18925 LUMO: 0.40001 factor:1 | -1 (0.92883) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42235 HOMO: -6.72121 LUMO: 0.19592 factor:1 | -1 (0.43677) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.46637 HOMO: -6.85999 LUMO: -0.39457 factor:1 | -1 (2.39275) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.05767 HOMO: -6.90625 LUMO: 0.05987 factor:1 | -1 (1.80145) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91318 HOMO: -7.00421 LUMO: 0.37552 factor:1 | -1 (1.94594) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.23150 HOMO: -6.56883 LUMO: -0.97689 factor:1 | -1 (1.62762) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30673 HOMO: -6.66679 LUMO: 0.56055 factor:1 | -1 (0.55239) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.14056 HOMO: -6.75931 LUMO: 0.32926 factor:1 | -1 (2.71855) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.90485 HOMO: -6.53617 LUMO: -1.06397 factor:1 | -1 (1.95427) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37099 HOMO: -6.78108 LUMO: 0.42722 factor:1 | 1 (-0.51187) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.54522 HOMO: -7.05319 LUMO: 0.61498 factor:1 | 1 (-0.68611) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20625 HOMO: -6.78380 LUMO: 1.49391 factor:1 | 1 (-0.34714) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59751 HOMO: -7.21102 LUMO: 0.27211 factor:1 | -1 (0.26161) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01099 HOMO: -6.67223 LUMO: 0.81362 factor:1 | -1 (0.84812) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14792 HOMO: -6.69944 LUMO: 1.40683 factor:1 | -1 (0.71120) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86274 HOMO: -7.02598 LUMO: 1.46941 factor:1 | -1 (0.99637) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25772 HOMO: -5.85045 LUMO: -0.76736 factor:1 | -1 (0.60140) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.03201 HOMO: -6.53890 LUMO: -0.50885 factor:1 | -1 (1.82711) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.97563 HOMO: -6.42733 LUMO: -0.63947 factor:1 | -1 (1.88349) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.22633 HOMO: -6.82189 LUMO: -0.85444 factor:1 | 1 (-0.36722) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33554 HOMO: -6.97428 LUMO: -1.22179 factor:1 | -1 (0.52357) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39992 HOMO: -6.93346 LUMO: -1.09934 factor:1 | 1 (-0.54080) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46159 HOMO: -7.17292 LUMO: -1.11839 factor:1 | -1 (0.39753) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10089 HOMO: -7.00965 LUMO: -1.23268 factor:1 | 1 (-0.24177) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18751 HOMO: -6.73210 LUMO: -1.12383 factor:1 | -1 (0.67160) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.64349 HOMO: -7.61375 LUMO: -0.11973 factor:1 | -1 (0.21562) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.34156 HOMO: -7.42327 LUMO: 0.41906 factor:1 | -1 (0.51756) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10810 HOMO: -6.94162 LUMO: -1.01771 factor:1 | 1 (-0.24898) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.87647 HOMO: -6.82189 LUMO: -0.92791 factor:1 | 1 (-1.01735) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23091 HOMO: -6.92258 LUMO: -1.73881 factor:1 | 1 (-0.37179) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97920 HOMO: -6.50896 LUMO: -1.60819 factor:1 | 1 (-0.12008) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20281 HOMO: -6.38379 LUMO: -2.18780 factor:1 | -1 (1.65630) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.03672 HOMO: -6.48992 LUMO: -0.97417 factor:1 | -1 (1.82240) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.34833 HOMO: -6.01644 LUMO: -0.04354 factor:1 | -1 (0.51078) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00824 HOMO: -6.70761 LUMO: -0.14422 factor:1 | -1 (0.85087) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.72349 HOMO: -6.70216 LUMO: 0.14422 factor:1 | -1 (2.13563) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.86183 HOMO: -7.07224 LUMO: -0.10885 factor:1 | -1 (1.99729) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33374 HOMO: -7.52667 LUMO: -0.74287 factor:1 | 1 (-0.47462) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07267 HOMO: -6.48447 LUMO: -0.96056 factor:1 | 1 (-0.21355) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37036 HOMO: -6.22597 LUMO: -0.41361 factor:1 | 1 (-0.51125) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.91688 HOMO: -6.12256 LUMO: -1.05852 factor:1 | 1 (-1.05776) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89904 HOMO: -6.97428 LUMO: -0.60681 factor:1 | 1 (-0.03992) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13499 HOMO: -6.78380 LUMO: -0.88981 factor:1 | 1 (-0.27587) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73158 HOMO: -6.85999 LUMO: 0.07891 factor:1 | -1 (0.12754) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10204 HOMO: -7.08312 LUMO: -0.60137 factor:1 | -1 (0.75708) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88212 HOMO: -6.57699 LUMO: -0.68028 factor:1 | -1 (0.97700) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93741 HOMO: -6.09807 LUMO: -0.31837 factor:1 | -1 (0.92170) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.20558 HOMO: -6.10624 LUMO: 0.14966 factor:1 | -1 (0.65354) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03282 HOMO: -6.77019 LUMO: -0.95784 factor:1 | -1 (0.82630) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77001 HOMO: -5.93208 LUMO: -0.44627 factor:1 | -1 (1.08911) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80114 HOMO: -6.12256 LUMO: -0.27756 factor:1 | -1 (1.05798) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12433 HOMO: -5.98106 LUMO: -0.37824 factor:1 | -1 (0.73479) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78881 HOMO: -7.06408 LUMO: -1.12927 factor:1 | -1 (1.07031) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.69504 HOMO: -6.70761 LUMO: -0.98505 factor:1 | -1 (1.16408) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02789 HOMO: -7.00965 LUMO: -0.42722 factor:1 | -1 (0.83123) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90601 HOMO: -5.96201 LUMO: -0.59049 factor:1 | -1 (0.95311) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.38239 HOMO: -6.34570 LUMO: -1.68438 factor:1 | 1 (-0.52327) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.12173 HOMO: -6.97156 LUMO: -1.85854 factor:1 | 1 (-1.26261) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18598 HOMO: -5.91848 LUMO: -2.51433 factor:1 | 1 (-0.32686) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87199 HOMO: -6.39195 LUMO: -1.66262 factor:1 | 1 (-0.01287) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68464 HOMO: -6.50352 LUMO: 0.19592 factor:1 | -1 (0.17448) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91944 HOMO: -6.45998 LUMO: 0.34831 factor:1 | -1 (1.93968) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10888 HOMO: -7.05319 LUMO: 0.23402 factor:1 | -1 (1.75024) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05801 HOMO: -6.61237 LUMO: 0.18232 factor:1 | 1 (-0.19889) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84554 HOMO: -6.57427 LUMO: 0.40545 factor:1 | -1 (0.01358) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.99451 HOMO: -7.26544 LUMO: 0.41089 factor:1 | -1 (1.86461) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.11854 HOMO: -6.26406 LUMO: -0.85444 factor:1 | -1 (1.74058) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.96888 HOMO: -6.25318 LUMO: -0.79457 factor:1 | -1 (1.89024) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80683 HOMO: -6.68040 LUMO: 0.41089 factor:1 | -1 (1.05229) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96079 HOMO: -6.37835 LUMO: 0.37280 factor:1 | -1 (0.89833) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85243 HOMO: -6.56067 LUMO: 0.62858 factor:1 | -1 (1.00669) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.40030 HOMO: -6.74026 LUMO: -0.04082 factor:1 | 1 (-0.54118) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.88844 HOMO: -6.53617 LUMO: 0.35103 factor:1 | 1 (-1.02933) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.04258 HOMO: -6.51985 LUMO: 0.25851 factor:1 | 1 (-0.18346) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.63416 HOMO: -6.58788 LUMO: -1.98371 factor:1 | -1 (0.22496) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79069 HOMO: -6.51441 LUMO: 0.29116 factor:1 | -1 (1.06843) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05736 HOMO: -6.81101 LUMO: 0.35647 factor:1 | -1 (0.80176) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71506 HOMO: -6.42733 LUMO: 0.10340 factor:1 | -1 (0.14406) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.66134 HOMO: -6.70761 LUMO: 0.28028 factor:1 | 1 (-0.80222) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74877 HOMO: -6.67495 LUMO: 0.01633 factor:1 | -1 (0.11034) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.00562 HOMO: -6.75387 LUMO: 0.15510 factor:1 | 1 (-0.14651) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.54778 HOMO: -6.56067 LUMO: 0.35919 factor:1 | 1 (-0.68867) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83193 HOMO: -7.16748 LUMO: 0.21497 factor:1 | -1 (0.02718) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79152 HOMO: -6.71849 LUMO: 0.26667 factor:1 | -1 (0.06759) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97218 HOMO: -6.69128 LUMO: 0.55783 factor:1 | 1 (-0.11306) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19140 HOMO: -6.71305 LUMO: 0.45987 factor:1 | -1 (0.66771) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35192 HOMO: -5.90487 LUMO: -0.70750 factor:1 | -1 (0.50719) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27606 HOMO: -6.84638 LUMO: -0.72110 factor:1 | -1 (0.58306) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96805 HOMO: -6.66135 LUMO: -1.13471 factor:1 | -1 (0.89106) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.63879 HOMO: -6.74026 LUMO: -0.64763 factor:1 | -1 (0.22033) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73667 HOMO: -6.69672 LUMO: -1.05036 factor:1 | -1 (0.12245) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.50237 HOMO: -6.78924 LUMO: -1.03675 factor:1 | 1 (-0.64325) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52520 HOMO: -6.81373 LUMO: -0.85988 factor:1 | 1 (-0.66608) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68986 HOMO: -7.26544 LUMO: 0.91158 factor:1 | -1 (0.16925) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24946 HOMO: -6.64230 LUMO: -1.92929 factor:1 | 1 (-0.39035) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.43285 HOMO: -7.20830 LUMO: 0.11429 factor:1 | -1 (0.42627) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22722 HOMO: -7.17020 LUMO: 0.04898 factor:1 | -1 (1.63189) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32290 HOMO: -7.16476 LUMO: 0.04898 factor:1 | -1 (1.53622) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.74735 HOMO: -6.59332 LUMO: -0.49253 factor:1 | -1 (2.11177) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.95089 HOMO: -7.46953 LUMO: 0.84083 factor:1 | -1 (1.90823) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.15899 HOMO: -7.39878 LUMO: 0.88709 factor:1 | -1 (2.70013) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.46275 HOMO: -6.84094 LUMO: -0.61498 factor:1 | -1 (2.39637) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.58041 HOMO: -6.03549 LUMO: -0.27211 factor:1 | -1 (2.27871) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12519.95817 HOMO: -7.31170 LUMO: -0.64763 factor:1 | -1 (2.90095) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.76474 HOMO: -6.88992 LUMO: -0.84627 factor:1 | -1 (2.09438) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.69033 HOMO: -7.12666 LUMO: -0.09252 factor:1 | -1 (1.16878) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52715 HOMO: -6.70489 LUMO: -0.63675 factor:1 | -1 (1.33197) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22268 HOMO: -6.98788 LUMO: 0.86804 factor:1 | -1 (1.63644) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.25642 HOMO: -6.80285 LUMO: -0.60954 factor:1 | -1 (1.60270) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36867 HOMO: -7.02054 LUMO: -0.74287 factor:1 | -1 (1.49045) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.06727 HOMO: -7.03686 LUMO: -0.81090 factor:1 | -1 (1.79184) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.41313 HOMO: -6.70489 LUMO: -1.00954 factor:1 | -1 (1.44599) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91459 HOMO: -7.69810 LUMO: 0.00544 factor:1 | -1 (1.94453) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12621 HOMO: -6.83550 LUMO: -0.11157 factor:1 | -1 (1.73290) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24186 HOMO: -6.76203 LUMO: -2.13609 factor:1 | -1 (1.61725) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.04869 HOMO: -6.72121 LUMO: -2.62862 factor:1 | -1 (1.81043) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.78368 HOMO: -6.48719 LUMO: -2.73474 factor:1 | -1 (2.07544) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34143 HOMO: -6.83006 LUMO: -0.00544 factor:1 | -1 (1.51769) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.65409 HOMO: -6.84094 LUMO: -1.11022 factor:1 | -1 (1.20503) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.75327 HOMO: -6.66951 LUMO: -1.23812 factor:1 | -1 (1.10584) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39299 HOMO: -6.78380 LUMO: -1.27894 factor:1 | -1 (1.46612) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78699 HOMO: -6.50352 LUMO: -0.56055 factor:1 | -1 (1.07213) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91513 HOMO: -7.77974 LUMO: -0.26395 factor:1 | -1 (0.94399) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48183 HOMO: -7.01510 LUMO: -1.64085 factor:1 | -1 (0.37729) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57239 HOMO: -6.59876 LUMO: -0.91158 factor:1 | -1 (0.28673) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75835 HOMO: -4.67219 LUMO: -0.67756 factor:1 | -1 (0.10076) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58996 HOMO: -6.70489 LUMO: -0.65579 factor:1 | 1 (-0.73084) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.53565 HOMO: -6.62325 LUMO: -0.60409 factor:1 | 1 (-0.67653) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69680 HOMO: -6.20147 LUMO: 0.15238 factor:1 | -1 (0.16232) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41922 HOMO: -6.43549 LUMO: -0.07075 factor:1 | -1 (0.43990) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53179 HOMO: -7.02054 LUMO: 0.13061 factor:1 | -1 (0.32733) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75865 HOMO: -7.04503 LUMO: 0.30749 factor:1 | -1 (0.10046) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73710 HOMO: -6.74842 LUMO: -0.99594 factor:1 | -1 (0.12202) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61745 HOMO: -6.35658 LUMO: 0.41633 factor:1 | -1 (0.24166) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30879 HOMO: -6.79740 LUMO: 0.56872 factor:1 | -1 (0.55032) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53174 HOMO: -6.51713 LUMO: -0.05987 factor:1 | -1 (0.32738) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.37905 HOMO: -6.68040 LUMO: 0.34558 factor:1 | -1 (0.48006) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42733 HOMO: -6.39740 LUMO: 0.50069 factor:1 | -1 (0.43179) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31301 HOMO: -6.91713 LUMO: -0.97145 factor:1 | -1 (0.54611) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30907 HOMO: -7.10761 LUMO: -0.27483 factor:1 | -1 (0.55005) | 1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40817 HOMO: -6.98788 LUMO: 0.40273 factor:1 | -1 (0.45095) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54755 HOMO: -6.87087 LUMO: 0.28572 factor:1 | -1 (0.31157) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.20281 HOMO: -7.36612 LUMO: -0.12245 factor:1 | -1 (0.65631) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34948 HOMO: -6.72938 LUMO: 0.33742 factor:1 | -1 (1.50963) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12768 HOMO: -7.32531 LUMO: 0.07619 factor:1 | -1 (1.73143) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12474 HOMO: -6.87087 LUMO: -0.08436 factor:1 | -1 (1.73437) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83395 HOMO: -6.67495 LUMO: 0.85988 factor:1 | -1 (0.02517) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58820 HOMO: -6.96339 LUMO: 0.65307 factor:1 | -1 (0.27092) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28184 HOMO: -6.58516 LUMO: -0.78641 factor:1 | -1 (1.57728) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26004 HOMO: -6.56883 LUMO: 0.44355 factor:1 | -1 (1.59908) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68183 HOMO: -6.68312 LUMO: 0.43538 factor:1 | -1 (0.17728) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30994 HOMO: -6.81917 LUMO: 0.20681 factor:1 | -1 (0.54918) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76053 HOMO: -6.91169 LUMO: 0.08163 factor:1 | -1 (0.09859) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42861 HOMO: -4.88444 LUMO: -0.49253 factor:1 | -1 (0.43051) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18885 HOMO: -6.42189 LUMO: 0.64763 factor:1 | -1 (0.67027) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.50170 HOMO: -6.24501 LUMO: 0.55783 factor:1 | -1 (1.35741) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36208 HOMO: -6.41372 LUMO: 0.29388 factor:1 | -1 (1.49703) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.47719 HOMO: -5.67902 LUMO: 1.77690 factor:1 | -1 (1.38193) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.14836 HOMO: -6.55794 LUMO: 0.05170 factor:1 | -1 (1.71075) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.27950 HOMO: -6.52801 LUMO: 0.25851 factor:1 | -1 (1.57962) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20603 HOMO: -7.08857 LUMO: 0.11157 factor:1 | -1 (1.65309) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.41621 HOMO: -6.58243 LUMO: 0.75648 factor:1 | -1 (1.44291) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.47961 HOMO: -7.22190 LUMO: 0.45171 factor:1 | -1 (1.37951) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.72666 HOMO: -6.47087 LUMO: 0.00000 factor:1 | -1 (1.13246) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01263 HOMO: -6.78652 LUMO: 1.32247 factor:1 | -1 (0.84649) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25663 HOMO: -6.74026 LUMO: 1.45309 factor:1 | -1 (0.60249) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33117 HOMO: -6.69944 LUMO: 0.76464 factor:1 | -1 (1.52795) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39381 HOMO: -6.62325 LUMO: 0.64763 factor:1 | -1 (1.46531) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.25571 HOMO: -6.45182 LUMO: 0.49253 factor:1 | -1 (1.60340) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.52382 HOMO: -7.14843 LUMO: 0.62586 factor:1 | -1 (0.33530) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25768 HOMO: -6.87087 LUMO: 1.53200 factor:1 | 1 (-0.39857) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.11313 HOMO: -6.54978 LUMO: 0.45171 factor:1 | 1 (-1.25401) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.87350 HOMO: -6.63686 LUMO: 0.80001 factor:1 | 1 (-1.01439) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.45047 HOMO: -7.00693 LUMO: 1.56193 factor:1 | 1 (-1.59135) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.17819 HOMO: -6.02460 LUMO: 1.72792 factor:1 | 1 (-1.31907) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.99620 HOMO: -6.36746 LUMO: -1.20002 factor:1 | 1 (-1.13708) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30568 HOMO: -7.26816 LUMO: -1.06397 factor:1 | 1 (-0.44657) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.13141 HOMO: -7.34707 LUMO: -1.09662 factor:1 | 1 (-1.27230) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.64781 HOMO: -7.93212 LUMO: -0.13606 factor:1 | 1 (-0.78869) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39929 HOMO: -6.80285 LUMO: 0.58504 factor:1 | 1 (-0.54017) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36211 HOMO: -7.12938 LUMO: 0.32926 factor:1 | -1 (1.49701) | 1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34856 HOMO: -6.86815 LUMO: -1.30070 factor:1 | -1 (1.51056) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33479 HOMO: -6.99333 LUMO: -1.03947 factor:1 | -1 (1.52433) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99083 HOMO: -7.56749 LUMO: -0.11157 factor:1 | -1 (0.86829) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26240 HOMO: -7.57293 LUMO: -0.07891 factor:1 | -1 (0.59672) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24847 HOMO: -7.30626 LUMO: 0.27211 factor:1 | -1 (0.61065) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85934 HOMO: -7.77974 LUMO: 0.27211 factor:1 | -1 (0.99977) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36980 HOMO: -7.11578 LUMO: 0.19864 factor:1 | -1 (0.48932) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06710 HOMO: -7.71171 LUMO: 0.57688 factor:1 | -1 (0.79201) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91749 HOMO: -7.83688 LUMO: 0.37824 factor:1 | -1 (0.94162) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22931 HOMO: -6.94979 LUMO: -1.66534 factor:1 | -1 (0.62981) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85964 HOMO: -6.97156 LUMO: -1.13199 factor:1 | -1 (0.99947) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.96638 HOMO: -6.91441 LUMO: -1.08301 factor:1 | 1 (-1.10726) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06084 HOMO: -6.71849 LUMO: -0.74831 factor:1 | 1 (-0.20172) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24315 HOMO: -7.09401 LUMO: -1.77690 factor:1 | 1 (-0.38403) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.99555 HOMO: -6.97156 LUMO: -1.45037 factor:1 | 1 (-1.13643) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.99911 HOMO: -7.22462 LUMO: -1.11295 factor:1 | 1 (-1.13999) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12503 HOMO: -7.85321 LUMO: 0.16599 factor:1 | 1 (-0.26591) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.64798 HOMO: -7.71987 LUMO: 0.55511 factor:1 | 1 (-0.78886) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72741 HOMO: -7.63551 LUMO: 0.14422 factor:1 | -1 (0.13170) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18712 HOMO: -6.98788 LUMO: -0.80546 factor:1 | 1 (-0.32801) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.38773 HOMO: -6.98788 LUMO: -1.16737 factor:1 | 1 (-0.52861) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44825 HOMO: -6.56611 LUMO: -1.60819 factor:1 | -1 (0.41086) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33481 HOMO: -6.95251 LUMO: 0.66396 factor:1 | -1 (0.52431) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30591 HOMO: -7.35252 LUMO: 0.49797 factor:1 | -1 (0.55321) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01121 HOMO: -6.90897 LUMO: -0.81090 factor:1 | -1 (0.84791) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.52251 HOMO: -7.04503 LUMO: -1.08301 factor:1 | -1 (0.33660) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10285 HOMO: -6.92530 LUMO: -1.29526 factor:1 | 1 (-0.24373) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32762 HOMO: -6.93074 LUMO: -1.25444 factor:1 | -1 (0.53149) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10093 HOMO: -6.73482 LUMO: -0.62042 factor:1 | -1 (0.75819) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33230 HOMO: -7.67633 LUMO: 0.59593 factor:1 | -1 (0.52681) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12519.99125 HOMO: -7.39061 LUMO: -0.19320 factor:1 | -1 (2.86786) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12519.98821 HOMO: -7.55388 LUMO: -0.20136 factor:1 | -1 (2.87091) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.57839 HOMO: -7.14027 LUMO: -0.99866 factor:1 | -1 (2.28072) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.86689 HOMO: -6.75931 LUMO: -0.73199 factor:1 | -1 (1.99223) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.54065 HOMO: -5.45044 LUMO: -0.18776 factor:1 | 1 (-0.68154) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35647 HOMO: -6.70761 LUMO: -0.84083 factor:1 | -1 (0.50265) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57089 HOMO: -6.05453 LUMO: -1.06669 factor:1 | -1 (0.28822) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16808 HOMO: -6.86815 LUMO: -0.98233 factor:1 | -1 (0.69103) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00014 HOMO: -6.73210 LUMO: -0.95240 factor:1 | -1 (0.85898) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19393 HOMO: -5.89671 LUMO: -1.05036 factor:1 | -1 (0.66518) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.87835 HOMO: -7.61102 LUMO: 0.33470 factor:1 | -1 (1.98077) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.04390 HOMO: -7.51034 LUMO: 0.23674 factor:1 | -1 (1.81522) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.00278 HOMO: -7.41510 LUMO: 0.62858 factor:1 | -1 (1.85633) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29219 HOMO: -6.76203 LUMO: -1.72792 factor:1 | 1 (-0.43307) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53242 HOMO: -6.60420 LUMO: -0.45715 factor:1 | -1 (0.32670) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03509 HOMO: -6.59060 LUMO: -0.58232 factor:1 | 1 (-0.17598) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22090 HOMO: -7.43687 LUMO: -0.76736 factor:1 | -1 (0.63822) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56942 HOMO: -6.08719 LUMO: -0.48708 factor:1 | -1 (0.28969) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32022 HOMO: -5.88854 LUMO: -0.05714 factor:1 | -1 (0.53889) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33835 HOMO: -7.34435 LUMO: -0.71838 factor:1 | -1 (0.52077) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32847 HOMO: -7.46408 LUMO: -0.63130 factor:1 | -1 (0.53065) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46436 HOMO: -7.00965 LUMO: -1.24900 factor:1 | -1 (0.39476) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13369 HOMO: -6.91169 LUMO: -0.88981 factor:1 | -1 (0.72543) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11336 HOMO: -6.78652 LUMO: -0.82178 factor:1 | -1 (0.74576) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26400 HOMO: -7.80423 LUMO: 0.87076 factor:1 | -1 (0.59511) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01551 HOMO: -6.97700 LUMO: -1.00954 factor:1 | -1 (0.84361) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14294 HOMO: -6.92530 LUMO: -0.88165 factor:1 | -1 (0.71618) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33297 HOMO: -7.14571 LUMO: -1.04492 factor:1 | -1 (1.52615) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.31362 HOMO: -7.49674 LUMO: 0.34558 factor:1 | -1 (1.54550) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29944 HOMO: -6.44094 LUMO: -1.20819 factor:1 | -1 (1.55968) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28584 HOMO: -6.47359 LUMO: -1.14016 factor:1 | -1 (1.57328) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.25239 HOMO: -6.61237 LUMO: -0.87076 factor:1 | -1 (1.60672) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10540 HOMO: -6.73754 LUMO: -1.09662 factor:1 | -1 (1.75372) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61168 HOMO: -6.97700 LUMO: 0.13061 factor:1 | -1 (0.24743) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60034 HOMO: -6.82734 LUMO: 0.59865 factor:1 | -1 (0.25878) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24716 HOMO: -6.86543 LUMO: -0.91430 factor:1 | -1 (0.61196) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29144 HOMO: -6.74298 LUMO: 0.28028 factor:1 | -1 (1.56768) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.90425 HOMO: -6.75387 LUMO: 0.19592 factor:1 | -1 (1.95487) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09919 HOMO: -7.05591 LUMO: 0.10612 factor:1 | -1 (1.75992) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.17898 HOMO: -6.86543 LUMO: 0.49253 factor:1 | -1 (1.68014) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69441 HOMO: -6.11440 LUMO: -1.12655 factor:1 | -1 (0.16471) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27225 HOMO: -6.77291 LUMO: -1.02859 factor:1 | -1 (0.58687) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71808 HOMO: -6.54978 LUMO: 0.29116 factor:1 | -1 (0.14104) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84035 HOMO: -7.18108 LUMO: 0.00000 factor:1 | -1 (1.01877) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07880 HOMO: -6.86271 LUMO: -1.15376 factor:1 | -1 (0.78031) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57528 HOMO: -6.78108 LUMO: -1.22723 factor:1 | -1 (0.28384) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77556 HOMO: -6.40828 LUMO: 0.02449 factor:1 | -1 (1.08356) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15622 HOMO: -6.43821 LUMO: 0.09796 factor:1 | -1 (0.70290) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96484 HOMO: -6.99877 LUMO: 0.40545 factor:1 | -1 (0.89427) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80110 HOMO: -6.68856 LUMO: 0.19320 factor:1 | -1 (0.05801) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57598 HOMO: -7.11034 LUMO: 0.31293 factor:1 | -1 (0.28313) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26346 HOMO: -6.92530 LUMO: -0.85444 factor:1 | -1 (0.59566) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07312 HOMO: -6.60148 LUMO: -0.59865 factor:1 | -1 (0.78600) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.70291 HOMO: -6.72938 LUMO: 0.30749 factor:1 | -1 (2.15620) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24352 HOMO: -7.31170 LUMO: 0.06803 factor:1 | -1 (1.61559) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.90101 HOMO: -7.09129 LUMO: -0.04626 factor:1 | -1 (1.95810) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18964 HOMO: -6.38379 LUMO: -0.76736 factor:1 | -1 (0.66948) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10776 HOMO: -6.13617 LUMO: -0.63947 factor:1 | -1 (0.75136) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25282 HOMO: -6.92258 LUMO: 0.37007 factor:1 | -1 (0.60630) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14299 HOMO: -6.35930 LUMO: 0.41361 factor:1 | -1 (0.71612) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95924 HOMO: -6.60420 LUMO: 0.26667 factor:1 | -1 (0.89988) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32969 HOMO: -6.04909 LUMO: 1.82588 factor:1 | -1 (0.52942) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71090 HOMO: -6.69672 LUMO: 1.72520 factor:1 | -1 (0.14822) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39152 HOMO: -6.50080 LUMO: 0.29116 factor:1 | -1 (0.46760) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86285 HOMO: -6.60692 LUMO: -0.43266 factor:1 | -1 (0.99626) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17864 HOMO: -6.93890 LUMO: 0.39729 factor:1 | -1 (0.68048) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67092 HOMO: -6.52801 LUMO: -0.47076 factor:1 | -1 (0.18819) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.85631 HOMO: -6.41100 LUMO: 0.30477 factor:1 | -1 (0.00280) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91014 HOMO: -6.37291 LUMO: -0.80001 factor:1 | 1 (-0.05102) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.82777 HOMO: -6.51985 LUMO: 1.44765 factor:1 | -1 (0.03135) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48360 HOMO: -6.64774 LUMO: 0.04626 factor:1 | -1 (0.37552) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.82774 HOMO: -6.65863 LUMO: 0.29933 factor:1 | -1 (0.03137) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80586 HOMO: -7.09673 LUMO: 0.28300 factor:1 | -1 (0.05325) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10880 HOMO: -6.57155 LUMO: -1.11567 factor:1 | -1 (1.75032) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21830 HOMO: -6.38379 LUMO: -0.60681 factor:1 | -1 (1.64082) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.83448 HOMO: -6.60148 LUMO: 0.18232 factor:1 | -1 (2.02464) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38478 HOMO: -6.96067 LUMO: -0.52246 factor:1 | -1 (1.47434) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91688 HOMO: -6.57427 LUMO: -0.84627 factor:1 | -1 (1.94224) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.75040 HOMO: -6.59332 LUMO: -0.98233 factor:1 | -1 (2.10872) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.96765 HOMO: -6.20692 LUMO: -0.27483 factor:1 | -1 (1.89146) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78579 HOMO: -6.81373 LUMO: 0.74559 factor:1 | -1 (1.07333) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16363 HOMO: -6.60420 LUMO: 0.54695 factor:1 | -1 (1.69549) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15362 HOMO: -6.58788 LUMO: -0.31021 factor:1 | -1 (1.70550) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39340 HOMO: -6.72938 LUMO: 0.64763 factor:1 | -1 (1.46571) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84914 HOMO: -6.86815 LUMO: 0.32109 factor:1 | -1 (1.00998) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.69807 HOMO: -6.63141 LUMO: 0.18776 factor:1 | -1 (2.16105) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79423 HOMO: -7.18653 LUMO: 0.09524 factor:1 | -1 (1.06489) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77575 HOMO: -6.83550 LUMO: 0.03537 factor:1 | -1 (1.08337) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86163 HOMO: -7.47769 LUMO: 0.40817 factor:1 | -1 (0.99749) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.57018 HOMO: -6.57971 LUMO: -0.63675 factor:1 | -1 (2.28894) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.78409 HOMO: -6.74842 LUMO: -0.16327 factor:1 | -1 (2.07503) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.64659 HOMO: -7.07224 LUMO: 0.61770 factor:1 | -1 (2.21253) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.78956 HOMO: -6.83006 LUMO: 0.54695 factor:1 | -1 (2.06956) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.57924 HOMO: -6.60148 LUMO: 1.23540 factor:1 | -1 (2.27988) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48007 HOMO: -6.99061 LUMO: 0.41089 factor:1 | -1 (1.37905) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.71986 HOMO: -6.63686 LUMO: 0.85172 factor:1 | -1 (1.13926) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.68832 HOMO: -6.50624 LUMO: 0.12517 factor:1 | -1 (1.17080) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80963 HOMO: -6.35658 LUMO: 0.36463 factor:1 | -1 (1.04949) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52282 HOMO: -6.34570 LUMO: 0.65035 factor:1 | -1 (1.33630) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24246 HOMO: -6.63141 LUMO: 1.25717 factor:1 | -1 (1.61666) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13242 HOMO: -6.91441 LUMO: 1.32792 factor:1 | -1 (1.72670) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39071 HOMO: -7.15387 LUMO: 0.64219 factor:1 | -1 (1.46841) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.47515 HOMO: -7.17836 LUMO: 0.60409 factor:1 | -1 (1.38397) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13343 HOMO: -6.92258 LUMO: 0.49525 factor:1 | -1 (1.72569) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34649 HOMO: -6.31032 LUMO: 0.48708 factor:1 | -1 (1.51263) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91880 HOMO: -6.49808 LUMO: 0.31021 factor:1 | -1 (0.94032) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17004 HOMO: -6.48447 LUMO: 0.37552 factor:1 | -1 (0.68907) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.70247 HOMO: -6.66135 LUMO: -1.08301 factor:1 | -1 (1.15665) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93322 HOMO: -6.33481 LUMO: -0.51974 factor:1 | -1 (0.92589) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94160 HOMO: -6.76475 LUMO: -0.15238 factor:1 | -1 (0.91751) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.76896 HOMO: -6.93346 LUMO: -0.10885 factor:1 | -1 (2.09016) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.98725 HOMO: -7.19741 LUMO: 0.73199 factor:1 | -1 (1.87187) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36067 HOMO: -6.82734 LUMO: 0.88437 factor:1 | -1 (1.49845) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43354 HOMO: -7.01237 LUMO: 0.02721 factor:1 | -1 (1.42558) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43852 HOMO: -6.39195 LUMO: 1.46941 factor:1 | -1 (1.42060) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38987 HOMO: -6.53890 LUMO: 1.32792 factor:1 | -1 (1.46925) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57327 HOMO: -6.82734 LUMO: 1.98099 factor:1 | -1 (1.28585) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22633 HOMO: -6.74570 LUMO: 1.68983 factor:1 | -1 (1.63279) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44930 HOMO: -6.41100 LUMO: 1.39050 factor:1 | -1 (1.40982) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13625 HOMO: -5.92664 LUMO: 1.65989 factor:1 | -1 (0.72287) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87992 HOMO: -6.07630 LUMO: 1.54833 factor:1 | -1 (0.97920) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27954 HOMO: -6.45998 LUMO: 0.68573 factor:1 | -1 (0.57958) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04751 HOMO: -6.52801 LUMO: 0.41361 factor:1 | -1 (0.81161) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.37865 HOMO: -6.77564 LUMO: 0.42178 factor:1 | -1 (0.48047) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.40431 HOMO: -6.56339 LUMO: 1.65717 factor:1 | -1 (1.45480) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13532 HOMO: -5.85861 LUMO: 1.90752 factor:1 | -1 (0.72380) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55790 HOMO: -6.77019 LUMO: -2.48440 factor:1 | -1 (1.30122) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82321 HOMO: -6.53890 LUMO: -1.82588 factor:1 | -1 (1.03591) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30137 HOMO: -6.50352 LUMO: -1.66806 factor:1 | -1 (0.55775) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57545 HOMO: -6.90625 LUMO: 0.43538 factor:1 | -1 (1.28367) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80040 HOMO: -6.85455 LUMO: 0.53062 factor:1 | -1 (1.05871) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.60731 HOMO: -6.49536 LUMO: 0.31021 factor:1 | -1 (1.25181) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83167 HOMO: -4.97696 LUMO: -0.09252 factor:1 | -1 (1.02745) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06465 HOMO: -5.31166 LUMO: 0.34286 factor:1 | -1 (0.79446) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02860 HOMO: -6.42461 LUMO: 0.74287 factor:1 | -1 (0.83052) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22449 HOMO: -6.59604 LUMO: 0.62858 factor:1 | -1 (0.63462) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27791 HOMO: -6.45998 LUMO: -0.61770 factor:1 | -1 (0.58121) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.64649 HOMO: -6.75659 LUMO: -0.34014 factor:1 | -1 (0.21263) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78986 HOMO: -6.63958 LUMO: 0.36191 factor:1 | -1 (0.06925) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75827 HOMO: -5.92936 LUMO: -0.67484 factor:1 | -1 (0.10085) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50164 HOMO: -5.67630 LUMO: 1.80956 factor:1 | -1 (0.35748) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42621 HOMO: -6.50352 LUMO: -0.78369 factor:1 | -1 (0.43291) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12842 HOMO: -6.35930 LUMO: -0.75648 factor:1 | -1 (1.73070) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13451 HOMO: -6.74298 LUMO: 0.48980 factor:1 | -1 (1.72460) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12891 HOMO: -6.85183 LUMO: 0.15510 factor:1 | -1 (1.73021) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09672 HOMO: -6.90897 LUMO: 0.26123 factor:1 | -1 (1.76240) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09557 HOMO: -6.85999 LUMO: 0.47892 factor:1 | -1 (1.76354) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.82395 HOMO: -6.69944 LUMO: 0.57416 factor:1 | -1 (2.03517) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29133 HOMO: -6.74026 LUMO: 0.69933 factor:1 | -1 (1.56778) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.41155 HOMO: -6.52801 LUMO: 0.75376 factor:1 | -1 (1.44756) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48810 HOMO: -7.05863 LUMO: 0.44627 factor:1 | -1 (1.37102) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38206 HOMO: -6.96339 LUMO: 0.48164 factor:1 | -1 (1.47706) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.95013 HOMO: -6.95795 LUMO: 0.44355 factor:1 | -1 (1.90899) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37615 HOMO: -6.36746 LUMO: 0.58777 factor:1 | -1 (1.48297) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30322 HOMO: -6.69400 LUMO: 0.40545 factor:1 | -1 (1.55589) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.08004 HOMO: -6.30760 LUMO: -0.66668 factor:1 | -1 (1.77908) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.99448 HOMO: -6.53617 LUMO: -0.64491 factor:1 | -1 (1.86463) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.64174 HOMO: -6.80829 LUMO: 0.17415 factor:1 | -1 (2.21737) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38494 HOMO: -6.80285 LUMO: 0.73471 factor:1 | -1 (1.47418) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.07364 HOMO: -6.43821 LUMO: 0.21769 factor:1 | -1 (1.78548) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24091 HOMO: -6.98788 LUMO: 0.10885 factor:1 | -1 (1.61821) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43403 HOMO: -7.15115 LUMO: 0.40817 factor:1 | -1 (1.42509) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.66144 HOMO: -6.00011 LUMO: -0.98505 factor:1 | -1 (1.19768) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16610 HOMO: -6.16882 LUMO: -0.77825 factor:1 | -1 (0.69302) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10242 HOMO: -6.30760 LUMO: 0.34831 factor:1 | -1 (0.75669) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11293 HOMO: -6.64502 LUMO: 0.63403 factor:1 | -1 (0.74619) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.76734 HOMO: -6.93618 LUMO: 0.96600 factor:1 | -1 (1.09178) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90438 HOMO: -6.45182 LUMO: 0.16327 factor:1 | -1 (0.95474) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83140 HOMO: -6.99605 LUMO: 0.20953 factor:1 | -1 (1.02772) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77567 HOMO: -6.72665 LUMO: 0.32654 factor:1 | -1 (1.08345) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.54625 HOMO: -6.38379 LUMO: 0.45443 factor:1 | -1 (1.31287) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.64500 HOMO: -6.65318 LUMO: 0.04354 factor:1 | -1 (1.21412) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.81880 HOMO: -6.94707 LUMO: -1.68438 factor:1 | -1 (1.04032) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93611 HOMO: -6.71849 LUMO: 0.15783 factor:1 | -1 (0.92301) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87099 HOMO: -6.97156 LUMO: 0.43266 factor:1 | -1 (0.98813) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28226 HOMO: -6.91441 LUMO: -0.54695 factor:1 | -1 (0.57685) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59685 HOMO: -6.74842 LUMO: -0.76192 factor:1 | -1 (0.26226) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.49753 HOMO: -6.70489 LUMO: 0.19048 factor:1 | -1 (0.36158) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28264 HOMO: -7.25728 LUMO: 0.33470 factor:1 | -1 (0.57647) | 1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59933 HOMO: -6.96339 LUMO: 0.55511 factor:1 | -1 (0.25979) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39603 HOMO: -6.77564 LUMO: 0.72382 factor:1 | -1 (0.46308) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08694 HOMO: -6.75387 LUMO: 0.39729 factor:1 | -1 (0.77218) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.57189 HOMO: -7.00149 LUMO: 0.06531 factor:1 | 1 (-0.71278) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69528 HOMO: -7.09945 LUMO: 0.33470 factor:1 | -1 (0.16384) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44295 HOMO: -7.20830 LUMO: 0.59593 factor:1 | -1 (0.41617) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30410 HOMO: -6.40556 LUMO: 0.56600 factor:1 | 1 (-0.44499) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60521 HOMO: -6.77291 LUMO: 0.73471 factor:1 | -1 (0.25391) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58257 HOMO: -6.65046 LUMO: 0.09796 factor:1 | -1 (0.27655) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38539 HOMO: -6.95795 LUMO: 0.22313 factor:1 | -1 (0.47372) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56417 HOMO: -6.85727 LUMO: 0.04626 factor:1 | -1 (0.29494) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58934 HOMO: -7.27360 LUMO: 0.42178 factor:1 | -1 (0.26977) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69413 HOMO: -6.78924 LUMO: -0.13334 factor:1 | -1 (0.16498) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28523 HOMO: -6.63141 LUMO: 0.38368 factor:1 | -1 (0.57389) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39241 HOMO: -6.92258 LUMO: 0.39184 factor:1 | -1 (0.46670) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30256 HOMO: -6.19331 LUMO: -0.46804 factor:1 | -1 (0.55655) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46583 HOMO: -7.26544 LUMO: -0.05442 factor:1 | -1 (0.39329) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41018 HOMO: -7.09401 LUMO: 0.30749 factor:1 | -1 (0.44893) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17611 HOMO: -6.14705 LUMO: -0.88709 factor:1 | -1 (0.68301) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14789 HOMO: -6.53617 LUMO: -0.28572 factor:1 | -1 (0.71122) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.81581 HOMO: -6.37291 LUMO: -0.67212 factor:1 | -1 (2.04330) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.72553 HOMO: -6.65591 LUMO: 0.03810 factor:1 | -1 (2.13359) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12842 HOMO: -7.11034 LUMO: 0.75103 factor:1 | -1 (1.73070) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.01106 HOMO: -6.85183 LUMO: -0.05987 factor:1 | -1 (1.84806) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.64194 HOMO: -6.70761 LUMO: -0.05442 factor:1 | -1 (0.21717) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31394 HOMO: -6.23413 LUMO: 0.06259 factor:1 | -1 (0.54518) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.72142 HOMO: -6.55794 LUMO: 0.74015 factor:1 | -1 (2.13770) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.03982 HOMO: -7.27905 LUMO: 0.26939 factor:1 | -1 (1.81930) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59707 HOMO: -6.34842 LUMO: -0.86804 factor:1 | -1 (0.26205) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60611 HOMO: -6.27222 LUMO: 1.46125 factor:1 | -1 (0.25301) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31415 HOMO: -6.65046 LUMO: 2.04902 factor:1 | -1 (0.54496) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80106 HOMO: -7.11850 LUMO: -1.14016 factor:1 | -1 (1.05806) | 1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04800 HOMO: -6.88720 LUMO: -1.20274 factor:1 | -1 (0.81112) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38154 HOMO: -6.69400 LUMO: -0.31565 factor:1 | -1 (1.47758) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22290 HOMO: -6.95523 LUMO: -1.55377 factor:1 | -1 (1.63622) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26619 HOMO: -6.41372 LUMO: -0.83539 factor:1 | -1 (1.59293) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.31169 HOMO: -6.13889 LUMO: -0.90070 factor:1 | -1 (1.54743) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.97179 HOMO: -6.44366 LUMO: -0.55511 factor:1 | -1 (1.88733) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.08839 HOMO: -6.10079 LUMO: -0.71022 factor:1 | -1 (1.77073) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.23130 HOMO: -6.90353 LUMO: -0.64763 factor:1 | -1 (1.62781) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26377 HOMO: -6.65046 LUMO: -0.82450 factor:1 | -1 (1.59535) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30820 HOMO: -6.81645 LUMO: -0.85444 factor:1 | -1 (0.55092) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40931 HOMO: -6.20692 LUMO: 1.30887 factor:1 | -1 (0.44980) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19854 HOMO: -5.96201 LUMO: 1.33880 factor:1 | -1 (1.66057) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.35161 HOMO: -6.52529 LUMO: 1.58914 factor:1 | -1 (1.50751) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06871 HOMO: -6.58516 LUMO: 1.97555 factor:1 | -1 (0.79041) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04452 HOMO: -6.84366 LUMO: 0.15783 factor:1 | -1 (0.81460) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07567 HOMO: -6.45726 LUMO: 0.42994 factor:1 | -1 (0.78344) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23423 HOMO: -6.75387 LUMO: 0.14422 factor:1 | -1 (0.62488) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.89606 HOMO: -6.69944 LUMO: 1.79051 factor:1 | 1 (-1.03694) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11518 HOMO: -6.59876 LUMO: 1.90208 factor:1 | 1 (-0.25606) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.88746 HOMO: -7.05863 LUMO: 1.20819 factor:1 | 1 (-1.02835) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58035 HOMO: -6.54978 LUMO: 2.01636 factor:1 | 1 (-0.72124) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.77128 HOMO: -5.52119 LUMO: 1.95106 factor:1 | -1 (0.08784) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02312 HOMO: -6.53617 LUMO: 1.60275 factor:1 | 1 (-0.16400) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.35826 HOMO: -6.11440 LUMO: 1.89119 factor:1 | 1 (-0.49914) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30741 HOMO: -7.31986 LUMO: 0.48708 factor:1 | -1 (0.55171) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08291 HOMO: -6.76475 LUMO: -0.75648 factor:1 | -1 (0.77620) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85461 HOMO: -6.76747 LUMO: -1.06941 factor:1 | -1 (1.00451) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55727 HOMO: -6.87087 LUMO: 0.72927 factor:1 | -1 (1.30185) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02626 HOMO: -7.00965 LUMO: 0.02177 factor:1 | -1 (0.83286) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.85138 HOMO: -6.54706 LUMO: -0.03265 factor:1 | -1 (2.00774) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.88790 HOMO: -6.62325 LUMO: -0.63675 factor:1 | -1 (1.97122) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19171 HOMO: -7.03414 LUMO: -1.24084 factor:1 | -1 (1.66740) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.07617 HOMO: -7.04503 LUMO: -0.10068 factor:1 | -1 (1.78294) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.86537 HOMO: -6.67223 LUMO: 0.03537 factor:1 | -1 (1.99375) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21824 HOMO: -6.82734 LUMO: 0.58777 factor:1 | -1 (1.64087) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.58871 HOMO: -6.84366 LUMO: 0.46531 factor:1 | -1 (2.27041) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.44783 HOMO: -7.03959 LUMO: -1.15104 factor:1 | -1 (2.41128) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.18450 HOMO: -6.91169 LUMO: -0.41361 factor:1 | -1 (1.67462) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34480 HOMO: -7.10217 LUMO: -0.44627 factor:1 | -1 (1.51431) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15830 HOMO: -6.88176 LUMO: -0.19592 factor:1 | -1 (1.70082) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22714 HOMO: -7.21374 LUMO: -0.46531 factor:1 | -1 (1.63198) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.06975 HOMO: -6.54978 LUMO: 0.16871 factor:1 | -1 (1.78937) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.14504 HOMO: -6.71305 LUMO: -0.13061 factor:1 | -1 (1.71407) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.00194 HOMO: -6.74842 LUMO: -0.36191 factor:1 | -1 (1.85718) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16994 HOMO: -6.74570 LUMO: -0.09796 factor:1 | -1 (1.68917) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.84000 HOMO: -6.93890 LUMO: -0.27211 factor:1 | -1 (2.01911) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22940 HOMO: -6.88720 LUMO: -0.18776 factor:1 | -1 (1.62972) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87594 HOMO: -6.74842 LUMO: 0.02993 factor:1 | -1 (0.98317) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52913 HOMO: -6.70216 LUMO: 0.01361 factor:1 | -1 (1.32998) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46840 HOMO: -6.90625 LUMO: 0.00544 factor:1 | -1 (1.39072) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.70008 HOMO: -6.18243 LUMO: 0.25851 factor:1 | -1 (1.15904) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.67206 HOMO: -6.32937 LUMO: -0.20953 factor:1 | -1 (2.18706) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.81837 HOMO: -6.78108 LUMO: 0.00544 factor:1 | -1 (2.04075) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.58835 HOMO: -5.97562 LUMO: 0.28572 factor:1 | -1 (2.27076) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.71219 HOMO: -5.97290 LUMO: -0.18504 factor:1 | -1 (2.14692) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.34840 HOMO: -6.12800 LUMO: 0.42178 factor:1 | -1 (2.51071) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.79644 HOMO: -6.24229 LUMO: -0.00816 factor:1 | -1 (2.06268) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.41063 HOMO: -6.61781 LUMO: 0.12789 factor:1 | -1 (1.44849) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45985 HOMO: -6.70489 LUMO: 0.14694 factor:1 | -1 (1.39926) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.22299 HOMO: -6.86543 LUMO: -0.21225 factor:1 | -1 (2.63613) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.26223 HOMO: -6.90081 LUMO: -0.20136 factor:1 | -1 (2.59689) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55009 HOMO: -7.12938 LUMO: -0.25851 factor:1 | -1 (1.30903) | 1 | 1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48652 HOMO: -6.93074 LUMO: -0.26667 factor:1 | -1 (1.37260) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.23831 HOMO: -7.00421 LUMO: -0.31021 factor:1 | -1 (2.62081) | -1 | -1 |
| G: -6258.49342 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.17224 HOMO: -7.10761 LUMO: -0.17415 factor:1 | -1 (2.68688) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12519.76121 HOMO: -8.21240 LUMO: 0.05987 factor:1 | -1 (3.09791) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12519.74943 HOMO: -7.14843 LUMO: -0.46531 factor:1 | -1 (3.10969) | 1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12519.98584 HOMO: -6.80829 LUMO: -0.29933 factor:1 | -1 (2.87328) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36091 HOMO: -6.84094 LUMO: -0.53606 factor:1 | -1 (1.49820) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46875 HOMO: -6.81917 LUMO: -0.26667 factor:1 | -1 (1.39037) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57346 HOMO: -6.85727 LUMO: -1.20002 factor:1 | -1 (1.28566) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58103 HOMO: -6.39468 LUMO: -1.06941 factor:1 | -1 (1.27809) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39675 HOMO: -6.00827 LUMO: -1.94017 factor:1 | -1 (1.46237) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22173 HOMO: -6.80829 LUMO: 0.18504 factor:1 | -1 (1.63739) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26886 HOMO: -6.54434 LUMO: -0.95784 factor:1 | -1 (1.59026) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32771 HOMO: -6.45454 LUMO: -0.07347 factor:1 | -1 (1.53140) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19694 HOMO: -5.33887 LUMO: 1.11839 factor:1 | -1 (1.66218) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.04793 HOMO: -5.75249 LUMO: 0.70477 factor:1 | -1 (1.81119) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.87606 HOMO: -5.64092 LUMO: 0.87076 factor:1 | -1 (1.98306) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.52231 HOMO: -5.14295 LUMO: 1.06124 factor:1 | -1 (2.33680) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.96232 HOMO: -5.05043 LUMO: 1.21091 factor:1 | -1 (1.89680) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92920 HOMO: -5.05588 LUMO: 1.02859 factor:1 | -1 (0.92992) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24115 HOMO: -5.76337 LUMO: 0.79457 factor:1 | -1 (0.61797) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44921 HOMO: -5.01506 LUMO: 1.00138 factor:1 | -1 (1.40990) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.72715 HOMO: -4.84363 LUMO: 1.53744 factor:1 | -1 (1.13197) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.59663 HOMO: -5.17833 LUMO: 1.45309 factor:1 | -1 (2.26249) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.65255 HOMO: -5.13751 LUMO: 0.51157 factor:1 | -1 (2.20657) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.55924 HOMO: -5.56473 LUMO: 0.32109 factor:1 | -1 (2.29988) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.36843 HOMO: -4.69941 LUMO: 1.14016 factor:1 | -1 (2.49069) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.93723 HOMO: -4.49260 LUMO: 1.86398 factor:1 | -1 (1.92189) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.82890 HOMO: -4.32117 LUMO: 1.68438 factor:1 | -1 (2.03021) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28263 HOMO: -4.44906 LUMO: 1.37690 factor:1 | -1 (1.57649) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37245 HOMO: -4.62049 LUMO: 1.34968 factor:1 | -1 (1.48667) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98441 HOMO: -4.59600 LUMO: 1.58370 factor:1 | -1 (0.87471) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24923 HOMO: -4.98785 LUMO: 1.46669 factor:1 | -1 (0.60989) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19440 HOMO: -5.06676 LUMO: 1.27349 factor:1 | -1 (0.66472) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41198 HOMO: -5.09125 LUMO: 1.13471 factor:1 | -1 (0.44714) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.81047 HOMO: -4.84635 LUMO: 1.33608 factor:1 | -1 (1.04865) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58247 HOMO: -4.94431 LUMO: 1.18370 factor:1 | -1 (1.27665) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53185 HOMO: -4.92526 LUMO: 1.39867 factor:1 | -1 (1.32726) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46959 HOMO: -5.71983 LUMO: 0.60137 factor:1 | -1 (1.38952) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82887 HOMO: -5.10486 LUMO: 1.05580 factor:1 | -1 (1.03025) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74184 HOMO: -5.20282 LUMO: 1.01226 factor:1 | -1 (1.11727) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45104 HOMO: -4.98513 LUMO: 1.53744 factor:1 | -1 (1.40808) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10738 HOMO: -5.67085 LUMO: 0.17687 factor:1 | -1 (1.75173) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78345 HOMO: -5.87222 LUMO: 0.12517 factor:1 | -1 (1.07567) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.42434 HOMO: -5.20826 LUMO: 0.91702 factor:1 | -1 (1.43477) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27369 HOMO: -5.94569 LUMO: 0.63130 factor:1 | -1 (0.58543) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45916 HOMO: -5.35792 LUMO: 0.91430 factor:1 | -1 (0.39995) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.45233 HOMO: -5.36336 LUMO: 1.44220 factor:1 | 1 (-0.59321) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61068 HOMO: -5.83412 LUMO: 0.71294 factor:1 | -1 (0.24844) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.54016 HOMO: -4.97696 LUMO: 1.72792 factor:1 | 1 (-0.68105) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47974 HOMO: -5.55929 LUMO: 0.23130 factor:1 | -1 (0.37938) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37858 HOMO: -5.71167 LUMO: 0.47348 factor:1 | 1 (-0.51947) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39815 HOMO: -7.31986 LUMO: -2.54699 factor:1 | 1 (-0.53903) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12405 HOMO: -5.34704 LUMO: 1.19730 factor:1 | 1 (-0.26493) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19010 HOMO: -5.45860 LUMO: 0.80818 factor:1 | -1 (0.66902) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30822 HOMO: -5.12663 LUMO: 1.20274 factor:1 | -1 (0.55089) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88647 HOMO: -5.37153 LUMO: 1.05580 factor:1 | -1 (0.97264) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44401 HOMO: -5.47221 LUMO: 0.97961 factor:1 | -1 (0.41511) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.93195 HOMO: -5.06948 LUMO: 1.12111 factor:1 | 1 (-1.07284) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.89900 HOMO: -5.19737 LUMO: 1.25444 factor:1 | 1 (-1.03988) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.98254 HOMO: -5.27901 LUMO: 1.00682 factor:1 | 1 (-1.12342) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.44698 HOMO: -5.38513 LUMO: 0.49253 factor:1 | 1 (-1.58787) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15485 HOMO: -5.12390 LUMO: 1.22995 factor:1 | 1 (-0.29573) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.74330 HOMO: -5.31438 LUMO: 0.70205 factor:1 | 1 (-0.88418) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.03043 HOMO: -5.17561 LUMO: 1.04492 factor:1 | 1 (-1.17131) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25072 HOMO: -4.94431 LUMO: 1.52656 factor:1 | 1 (-0.39160) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72581 HOMO: -5.13751 LUMO: 0.93879 factor:1 | -1 (0.13331) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67762 HOMO: -5.49942 LUMO: 0.97689 factor:1 | -1 (0.18150) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39013 HOMO: -5.79058 LUMO: 0.53879 factor:1 | -1 (0.46899) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40376 HOMO: -5.36881 LUMO: 1.56465 factor:1 | -1 (0.45536) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.29108 HOMO: -4.67492 LUMO: 1.32792 factor:1 | -1 (0.56804) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.43516 HOMO: -4.60145 LUMO: 1.19458 factor:1 | -1 (0.42395) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.04883 HOMO: -4.49260 LUMO: 1.60547 factor:1 | 1 (-1.18971) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25368 HOMO: -4.65043 LUMO: 1.34696 factor:1 | 1 (-0.39457) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.07400 HOMO: -4.77560 LUMO: 1.35241 factor:1 | 1 (-1.21488) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.18385 HOMO: -4.94431 LUMO: 1.17825 factor:1 | 1 (-1.32473) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33308 HOMO: -4.87084 LUMO: 1.41771 factor:1 | 1 (-0.47397) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.02298 HOMO: -5.34432 LUMO: 1.16737 factor:1 | 1 (-1.16386) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07460 HOMO: -4.94975 LUMO: 1.67622 factor:1 | 1 (-0.21549) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27254 HOMO: -4.81369 LUMO: 1.14288 factor:1 | 1 (-0.41342) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37452 HOMO: -5.22459 LUMO: 0.29660 factor:1 | -1 (1.48460) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16730 HOMO: -5.21642 LUMO: 0.37824 factor:1 | -1 (1.69181) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30456 HOMO: -5.00417 LUMO: 1.01226 factor:1 | -1 (1.55456) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19543 HOMO: -5.46677 LUMO: 0.10612 factor:1 | -1 (0.66369) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98688 HOMO: -5.51303 LUMO: 0.54151 factor:1 | -1 (0.87223) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25317 HOMO: -5.63004 LUMO: 0.17960 factor:1 | -1 (0.60594) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11018 HOMO: -4.79193 LUMO: 1.12111 factor:1 | -1 (0.74894) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85153 HOMO: -5.43411 LUMO: 0.45987 factor:1 | -1 (1.00758) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97635 HOMO: -7.06135 LUMO: -2.13881 factor:1 | -1 (0.88276) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07845 HOMO: -5.33071 LUMO: 1.14016 factor:1 | -1 (0.78067) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.22100 HOMO: -7.12394 LUMO: -0.03810 factor:1 | 1 (-0.36188) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.12845 HOMO: -7.20558 LUMO: -2.50889 factor:1 | 1 (-1.26933) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.18613 HOMO: -7.26816 LUMO: -2.11432 factor:1 | 1 (-1.32702) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.70961 HOMO: -7.89674 LUMO: 0.31021 factor:1 | 1 (-0.85049) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96208 HOMO: -7.26544 LUMO: 0.22858 factor:1 | 1 (-0.10297) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15469 HOMO: -7.12666 LUMO: -0.02449 factor:1 | 1 (-0.29557) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.34944 HOMO: -7.68722 LUMO: 0.71838 factor:1 | 1 (-0.49032) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57389 HOMO: -6.86271 LUMO: -0.96056 factor:1 | -1 (0.28523) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28907 HOMO: -7.07496 LUMO: -1.11839 factor:1 | -1 (1.57004) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11597 HOMO: -7.06952 LUMO: -2.08439 factor:1 | -1 (0.74314) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33824 HOMO: -6.60965 LUMO: -2.11977 factor:1 | -1 (0.52088) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92623 HOMO: -6.87360 LUMO: -1.85854 factor:1 | -1 (0.93289) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26936 HOMO: -7.67089 LUMO: -0.24762 factor:1 | -1 (0.58975) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54926 HOMO: -6.45726 LUMO: -1.86398 factor:1 | -1 (0.30986) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28270 HOMO: -6.91713 LUMO: 0.33198 factor:1 | -1 (0.57642) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93959 HOMO: -6.83278 LUMO: 0.26667 factor:1 | -1 (0.91953) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58608 HOMO: -6.89264 LUMO: -1.00682 factor:1 | -1 (0.27304) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38948 HOMO: -6.57427 LUMO: 0.22041 factor:1 | -1 (0.46964) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38616 HOMO: -7.52123 LUMO: -0.01905 factor:1 | -1 (0.47296) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61239 HOMO: -7.37429 LUMO: -0.08980 factor:1 | -1 (0.24673) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75329 HOMO: -7.28449 LUMO: -0.26395 factor:1 | -1 (0.10583) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26011 HOMO: -6.79740 LUMO: -0.60954 factor:1 | -1 (0.59900) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.51138 HOMO: -7.12666 LUMO: -0.60681 factor:1 | -1 (0.34773) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.52638 HOMO: -6.96611 LUMO: -0.30477 factor:1 | -1 (0.33274) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.43054 HOMO: -7.08040 LUMO: -0.31293 factor:1 | -1 (0.42858) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28116 HOMO: -6.78924 LUMO: -0.73743 factor:1 | -1 (1.57796) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.93492 HOMO: -7.57293 LUMO: -1.11295 factor:1 | -1 (1.92420) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.27778 HOMO: -7.15932 LUMO: -0.23130 factor:1 | -1 (1.58134) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67617 HOMO: -7.48585 LUMO: -0.10068 factor:1 | -1 (0.18294) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27347 HOMO: -7.17020 LUMO: -0.26123 factor:1 | -1 (0.58564) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47742 HOMO: -7.43143 LUMO: -0.16055 factor:1 | -1 (0.38169) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93477 HOMO: -7.14843 LUMO: -0.10612 factor:1 | -1 (0.92434) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24109 HOMO: -6.95523 LUMO: -0.22585 factor:1 | -1 (0.61802) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28558 HOMO: -7.06680 LUMO: -0.51974 factor:1 | -1 (0.57353) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.20602 HOMO: -6.80829 LUMO: -0.64763 factor:1 | -1 (0.65310) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92446 HOMO: -7.13210 LUMO: -0.48164 factor:1 | -1 (0.93466) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02356 HOMO: -7.16204 LUMO: -0.45715 factor:1 | -1 (0.83555) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74288 HOMO: -7.15115 LUMO: -0.43266 factor:1 | -1 (1.11624) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16985 HOMO: -7.15932 LUMO: -2.52794 factor:1 | -1 (0.68926) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44227 HOMO: -7.21102 LUMO: -2.65311 factor:1 | -1 (1.41684) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36690 HOMO: -6.57427 LUMO: -2.78645 factor:1 | -1 (1.49222) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.86376 HOMO: -6.40828 LUMO: -3.23815 factor:1 | -1 (1.99536) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15043 HOMO: -7.71987 LUMO: -0.20953 factor:1 | -1 (1.70868) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.47558 HOMO: -7.47769 LUMO: -0.43810 factor:1 | -1 (1.38354) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55945 HOMO: -6.68040 LUMO: -2.22589 factor:1 | -1 (1.29967) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74087 HOMO: -6.92802 LUMO: -1.99187 factor:1 | -1 (1.11825) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91254 HOMO: -7.73620 LUMO: 0.01633 factor:1 | -1 (0.94658) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39217 HOMO: -7.28721 LUMO: -0.18504 factor:1 | -1 (0.46695) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45666 HOMO: -7.49674 LUMO: -0.19864 factor:1 | -1 (0.40246) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02263 HOMO: -7.10489 LUMO: -2.56331 factor:1 | 1 (-0.16351) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02990 HOMO: -7.36612 LUMO: 0.16055 factor:1 | 1 (-0.17078) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24746 HOMO: -7.67633 LUMO: 0.33198 factor:1 | -1 (0.61166) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79479 HOMO: -7.07768 LUMO: -0.27483 factor:1 | -1 (0.06433) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.49862 HOMO: -7.32531 LUMO: 0.05442 factor:1 | -1 (0.36050) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13491 HOMO: -6.79740 LUMO: -1.21635 factor:1 | -1 (0.72420) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.29655 HOMO: -7.14027 LUMO: 0.12517 factor:1 | -1 (0.56257) | 1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99883 HOMO: -7.17292 LUMO: 0.16871 factor:1 | -1 (0.86029) | 1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28585 HOMO: -7.08312 LUMO: -1.38778 factor:1 | -1 (0.57326) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21506 HOMO: -6.75387 LUMO: -1.88031 factor:1 | -1 (1.64406) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29101 HOMO: -7.07768 LUMO: -1.25717 factor:1 | -1 (1.56811) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22760 HOMO: -6.46543 LUMO: -1.14016 factor:1 | -1 (1.63151) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15109 HOMO: -7.37973 LUMO: -0.45987 factor:1 | -1 (1.70803) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16891 HOMO: -7.46408 LUMO: 0.03265 factor:1 | -1 (1.69021) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.05182 HOMO: -7.96477 LUMO: -0.19864 factor:1 | -1 (1.80730) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45805 HOMO: -6.93890 LUMO: -1.11839 factor:1 | -1 (0.40107) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.01395 HOMO: -7.06408 LUMO: -1.08846 factor:1 | 1 (-0.15483) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74042 HOMO: -7.14027 LUMO: -0.33470 factor:1 | -1 (0.11870) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12012 HOMO: -7.38245 LUMO: 0.10885 factor:1 | -1 (1.73900) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69291 HOMO: -7.59470 LUMO: -1.21363 factor:1 | -1 (0.16621) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39290 HOMO: -7.23279 LUMO: -1.23812 factor:1 | -1 (0.46621) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48886 HOMO: -6.90897 LUMO: 0.23402 factor:1 | -1 (1.37026) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54763 HOMO: -7.36340 LUMO: -0.17143 factor:1 | -1 (0.31149) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78378 HOMO: -6.61781 LUMO: -0.01361 factor:1 | -1 (1.07534) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11225 HOMO: -6.80013 LUMO: 0.38368 factor:1 | -1 (0.74687) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15930 HOMO: -6.72121 LUMO: -0.95512 factor:1 | -1 (1.69981) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19441 HOMO: -6.24773 LUMO: -0.69933 factor:1 | -1 (1.66471) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.23299 HOMO: -6.56883 LUMO: 0.14694 factor:1 | -1 (1.62613) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.31601 HOMO: -6.51441 LUMO: -1.27621 factor:1 | -1 (1.54310) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15661 HOMO: -6.91986 LUMO: -1.16737 factor:1 | -1 (1.70251) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26423 HOMO: -6.17971 LUMO: -0.65307 factor:1 | -1 (1.59489) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38249 HOMO: -7.22462 LUMO: 0.04354 factor:1 | -1 (1.47663) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.99631 HOMO: -7.16204 LUMO: -0.23674 factor:1 | -1 (1.86281) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.27751 HOMO: -6.81645 LUMO: -0.19320 factor:1 | -1 (1.58161) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.97764 HOMO: -6.69400 LUMO: 0.04082 factor:1 | -1 (1.88148) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.18763 HOMO: -6.63141 LUMO: -0.22858 factor:1 | -1 (1.67149) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.03413 HOMO: -6.92258 LUMO: -1.11295 factor:1 | -1 (1.82499) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.14597 HOMO: -6.60148 LUMO: -1.13744 factor:1 | -1 (1.71315) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32722 HOMO: -6.78108 LUMO: -0.82450 factor:1 | -1 (1.53189) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32118 HOMO: -7.05591 LUMO: -0.97145 factor:1 | -1 (1.53793) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29762 HOMO: -6.65318 LUMO: -1.26261 factor:1 | -1 (1.56150) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.35191 HOMO: -6.98244 LUMO: -0.98233 factor:1 | -1 (1.50721) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10613 HOMO: -7.11850 LUMO: -0.99594 factor:1 | -1 (1.75298) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.99032 HOMO: -6.64230 LUMO: -0.93879 factor:1 | -1 (1.86880) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.11903 HOMO: -6.62053 LUMO: -1.22451 factor:1 | -1 (1.74009) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20641 HOMO: -7.02598 LUMO: -0.85172 factor:1 | -1 (1.65271) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.23065 HOMO: -7.06680 LUMO: -0.89253 factor:1 | -1 (1.62847) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84772 HOMO: -7.17292 LUMO: 0.00272 factor:1 | -1 (1.01139) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84225 HOMO: -7.03142 LUMO: -0.35103 factor:1 | -1 (1.01686) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95804 HOMO: -6.96884 LUMO: -0.09796 factor:1 | -1 (0.90108) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89110 HOMO: -6.56339 LUMO: -0.99322 factor:1 | -1 (0.96802) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32540 HOMO: -7.08857 LUMO: -0.17687 factor:1 | -1 (1.53372) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33860 HOMO: -7.05863 LUMO: -0.22041 factor:1 | -1 (1.52052) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.95103 HOMO: -7.15115 LUMO: -0.17960 factor:1 | -1 (1.90809) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20390 HOMO: -6.67495 LUMO: -0.96600 factor:1 | -1 (1.65521) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.66149 HOMO: -6.74026 LUMO: -1.79867 factor:1 | -1 (1.19763) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80655 HOMO: -6.73482 LUMO: -1.78235 factor:1 | -1 (1.05256) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.70359 HOMO: -6.09807 LUMO: 0.16871 factor:1 | -1 (1.15553) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.71211 HOMO: -6.72393 LUMO: 0.27211 factor:1 | -1 (2.14701) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.97443 HOMO: -6.40556 LUMO: -0.04354 factor:1 | -1 (1.88469) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19811 HOMO: -6.56883 LUMO: 0.22041 factor:1 | -1 (1.66101) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.99636 HOMO: -7.22462 LUMO: 0.15783 factor:1 | -1 (1.86276) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.41661 HOMO: -6.83550 LUMO: 0.19320 factor:1 | -1 (1.44250) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55313 HOMO: -7.26816 LUMO: -0.07619 factor:1 | -1 (1.30598) | 1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53368 HOMO: -7.13483 LUMO: 0.33198 factor:1 | -1 (1.32544) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.49403 HOMO: -6.58243 LUMO: -0.26395 factor:1 | -1 (1.36509) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02609 HOMO: -7.38517 LUMO: 0.17143 factor:1 | -1 (0.83302) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99331 HOMO: -6.80013 LUMO: 0.25851 factor:1 | -1 (0.86581) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91513 HOMO: -6.96611 LUMO: 0.11429 factor:1 | -1 (0.94399) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87646 HOMO: -6.51713 LUMO: -1.14560 factor:1 | -1 (0.98266) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96890 HOMO: -7.15387 LUMO: -0.35647 factor:1 | -1 (0.89022) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95948 HOMO: -5.26540 LUMO: 1.26805 factor:1 | -1 (0.89964) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82661 HOMO: -6.76475 LUMO: -0.16327 factor:1 | -1 (1.03251) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37893 HOMO: -6.55250 LUMO: -0.71838 factor:1 | -1 (1.48019) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.11280 HOMO: -6.76203 LUMO: -1.08301 factor:1 | -1 (1.74632) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.23784 HOMO: -7.14027 LUMO: -0.01633 factor:1 | -1 (1.62128) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36646 HOMO: -6.94979 LUMO: -0.93879 factor:1 | -1 (1.49265) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33119 HOMO: -6.74842 LUMO: 0.31293 factor:1 | -1 (0.52793) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36417 HOMO: -6.43821 LUMO: 0.05987 factor:1 | -1 (0.49495) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31282 HOMO: -6.60420 LUMO: 0.22585 factor:1 | -1 (0.54630) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57008 HOMO: -6.43821 LUMO: 0.05987 factor:1 | -1 (0.28904) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47103 HOMO: -6.34570 LUMO: 1.43948 factor:1 | -1 (0.38809) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55476 HOMO: -6.03004 LUMO: 1.21363 factor:1 | -1 (0.30436) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.63914 HOMO: -6.68040 LUMO: -0.92247 factor:1 | -1 (0.21998) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.37704 HOMO: -6.92530 LUMO: -0.31293 factor:1 | -1 (0.48208) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08550 HOMO: -6.94979 LUMO: -0.19864 factor:1 | -1 (0.77362) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04199 HOMO: -6.80829 LUMO: -0.30477 factor:1 | -1 (0.81713) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15048 HOMO: -7.22734 LUMO: -1.02859 factor:1 | -1 (0.70864) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82046 HOMO: -6.93890 LUMO: -0.72382 factor:1 | -1 (1.03866) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96307 HOMO: -7.27088 LUMO: -0.78097 factor:1 | -1 (0.89604) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06656 HOMO: -7.29809 LUMO: -0.97145 factor:1 | -1 (0.79256) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98599 HOMO: -7.18925 LUMO: -0.94696 factor:1 | -1 (0.87313) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.81549 HOMO: -7.33891 LUMO: -0.96873 factor:1 | 1 (-0.95637) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10105 HOMO: -7.36068 LUMO: -0.28028 factor:1 | 1 (-0.24194) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.81864 HOMO: -7.10761 LUMO: -1.14832 factor:1 | 1 (-0.95953) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14171 HOMO: -6.94707 LUMO: -0.65307 factor:1 | 1 (-0.28259) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10149 HOMO: -6.91713 LUMO: -1.81228 factor:1 | 1 (-0.24237) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.67225 HOMO: -6.78652 LUMO: -2.01636 factor:1 | 1 (-0.81313) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23156 HOMO: -6.52801 LUMO: -1.17553 factor:1 | 1 (-0.37244) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33581 HOMO: -7.54844 LUMO: -1.18642 factor:1 | 1 (-0.47669) | 1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.61559 HOMO: -7.52939 LUMO: -1.23812 factor:1 | 1 (-0.75648) | 1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.99361 HOMO: -7.94572 LUMO: -0.81634 factor:1 | 1 (-1.13450) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12756 HOMO: -7.55932 LUMO: -0.86260 factor:1 | 1 (-0.26844) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05330 HOMO: -7.72259 LUMO: -1.39050 factor:1 | 1 (-0.19418) | 1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.46797 HOMO: -7.11850 LUMO: -1.01498 factor:1 | 1 (-0.60885) | 1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11371 HOMO: -7.09673 LUMO: -1.00954 factor:1 | 1 (-0.25459) | 1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.67472 HOMO: -6.06270 LUMO: 0.16327 factor:1 | 1 (-0.81561) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15637 HOMO: -5.71167 LUMO: 0.70477 factor:1 | 1 (-0.29726) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18345 HOMO: -5.38241 LUMO: 0.86260 factor:1 | 1 (-0.32433) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15624 HOMO: -5.67357 LUMO: 1.27621 factor:1 | 1 (-0.29712) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96666 HOMO: -7.56204 LUMO: -0.68573 factor:1 | 1 (-0.10754) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79786 HOMO: -5.57833 LUMO: 1.13199 factor:1 | -1 (0.06125) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06176 HOMO: -7.58653 LUMO: -0.66124 factor:1 | 1 (-0.20264) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.28400 HOMO: -7.91851 LUMO: -1.10206 factor:1 | 1 (-0.42488) | 1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24877 HOMO: -6.48992 LUMO: -1.00138 factor:1 | -1 (0.61035) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42425 HOMO: -7.09673 LUMO: -0.45171 factor:1 | -1 (0.43487) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.85906 HOMO: -6.63686 LUMO: 0.09252 factor:1 | -1 (0.00005) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93019 HOMO: -6.84366 LUMO: -0.14422 factor:1 | 1 (-0.07108) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93368 HOMO: -6.93074 LUMO: 0.04354 factor:1 | 1 (-0.07456) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91686 HOMO: -6.90353 LUMO: -0.19864 factor:1 | 1 (-0.05774) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55544 HOMO: -6.59876 LUMO: -0.10068 factor:1 | -1 (0.30368) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83925 HOMO: -6.74570 LUMO: -0.44627 factor:1 | -1 (0.01986) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.86527 HOMO: -6.60148 LUMO: -0.61770 factor:1 | 1 (-0.00615) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73601 HOMO: -6.55794 LUMO: -1.06941 factor:1 | -1 (0.12310) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.34088 HOMO: -7.12666 LUMO: -0.11973 factor:1 | -1 (0.51824) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33318 HOMO: -7.21646 LUMO: -0.50069 factor:1 | -1 (0.52594) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16066 HOMO: -7.27632 LUMO: -1.00682 factor:1 | -1 (0.69846) | 1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15519 HOMO: -6.74298 LUMO: 0.04354 factor:1 | -1 (0.70393) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31312 HOMO: -6.37291 LUMO: 0.14150 factor:1 | -1 (0.54600) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26166 HOMO: -5.61371 LUMO: 1.28438 factor:1 | -1 (0.59745) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08972 HOMO: -5.52119 LUMO: 0.99866 factor:1 | -1 (0.76940) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24419 HOMO: -6.51985 LUMO: -0.10885 factor:1 | -1 (0.61492) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38554 HOMO: -5.61371 LUMO: 0.77280 factor:1 | -1 (1.47358) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.93339 HOMO: -5.58922 LUMO: 0.24490 factor:1 | -1 (1.92572) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09634 HOMO: -6.32665 LUMO: -0.57144 factor:1 | -1 (1.76278) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.11035 HOMO: -6.29127 LUMO: -0.93607 factor:1 | -1 (1.74877) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.98825 HOMO: -5.49670 LUMO: 0.27211 factor:1 | -1 (1.87086) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13435 HOMO: -5.68990 LUMO: 0.24218 factor:1 | -1 (1.72477) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30709 HOMO: -5.68174 LUMO: 0.69933 factor:1 | -1 (1.55203) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.08537 HOMO: -5.28173 LUMO: 1.00954 factor:1 | -1 (1.77375) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42297 HOMO: -5.94025 LUMO: 0.73471 factor:1 | -1 (0.43614) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33984 HOMO: -5.65725 LUMO: 1.28710 factor:1 | -1 (0.51927) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11976 HOMO: -5.41507 LUMO: 0.87076 factor:1 | -1 (0.73936) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.85617 HOMO: -5.96474 LUMO: 0.29660 factor:1 | -1 (2.00295) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.04330 HOMO: -7.00421 LUMO: 0.08708 factor:1 | -1 (1.81582) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.07617 HOMO: -5.40418 LUMO: 0.90070 factor:1 | -1 (1.78294) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75152 HOMO: -7.00421 LUMO: -0.30477 factor:1 | -1 (0.10759) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53432 HOMO: -5.85861 LUMO: 0.74015 factor:1 | -1 (0.32480) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90451 HOMO: -5.71439 LUMO: 0.26395 factor:1 | -1 (0.95460) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72589 HOMO: -7.13755 LUMO: -0.78369 factor:1 | -1 (0.13323) | 1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01573 HOMO: -7.31442 LUMO: -0.98233 factor:1 | -1 (0.84339) | 1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05162 HOMO: -7.25728 LUMO: -1.00410 factor:1 | -1 (0.80750) | 1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17366 HOMO: -7.48585 LUMO: -0.83811 factor:1 | -1 (0.68545) | 1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03652 HOMO: -7.24911 LUMO: -0.77280 factor:1 | -1 (0.82260) | 1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98569 HOMO: -7.55116 LUMO: -1.19730 factor:1 | -1 (0.87343) | 1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02408 HOMO: -5.76881 LUMO: 0.28028 factor:1 | -1 (0.83504) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98286 HOMO: -5.77153 LUMO: -0.26939 factor:1 | -1 (0.87626) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94084 HOMO: -5.82868 LUMO: 0.36735 factor:1 | -1 (0.91828) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99809 HOMO: -5.83140 LUMO: -0.17960 factor:1 | -1 (0.86102) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48807 HOMO: -6.28855 LUMO: 0.01088 factor:1 | -1 (1.37105) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99883 HOMO: -6.31576 LUMO: 0.25307 factor:1 | -1 (0.86029) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.70652 HOMO: -7.06408 LUMO: -2.76196 factor:1 | -1 (1.15259) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96571 HOMO: -5.95657 LUMO: 0.37552 factor:1 | -1 (0.89340) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16569 HOMO: -6.61781 LUMO: 0.02721 factor:1 | -1 (0.69343) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57245 HOMO: -6.26678 LUMO: -0.66668 factor:1 | -1 (1.28666) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00691 HOMO: -6.00011 LUMO: -0.13334 factor:1 | -1 (0.85221) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05717 HOMO: -5.60555 LUMO: 0.67484 factor:1 | -1 (0.80195) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74489 HOMO: -5.79875 LUMO: 0.99049 factor:1 | -1 (1.11422) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02057 HOMO: -5.97834 LUMO: 0.48436 factor:1 | -1 (0.83855) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74764 HOMO: -5.82868 LUMO: 0.91974 factor:1 | -1 (1.11148) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79363 HOMO: -5.86677 LUMO: 0.99594 factor:1 | -1 (1.06549) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97203 HOMO: -5.70079 LUMO: 0.48980 factor:1 | -1 (0.88709) | -1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36546 HOMO: -7.39605 LUMO: -1.02315 factor:1 | -1 (1.49366) | 1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02612 HOMO: -7.22734 LUMO: -1.12927 factor:1 | -1 (0.83299) | 1 | -1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.56636 HOMO: -7.58926 LUMO: -0.65035 factor:1 | -1 (1.29276) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94832 HOMO: -7.43959 LUMO: -0.75648 factor:1 | -1 (0.91079) | 1 | 1 |
| G: -6258.49342 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57482 HOMO: -7.55388 LUMO: -1.15104 factor:1 | -1 (1.28430) | 1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77689 HOMO: -6.74570 LUMO: -2.85447 factor:1 | -1 (1.08222) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88808 HOMO: -7.35524 LUMO: -1.25444 factor:1 | -1 (0.97104) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91505 HOMO: -6.81645 LUMO: -1.20819 factor:1 | -1 (0.94407) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83306 HOMO: -6.99605 LUMO: -1.62996 factor:1 | -1 (1.02606) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94492 HOMO: -6.88992 LUMO: -0.47620 factor:1 | -1 (0.91419) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36115 HOMO: -7.22190 LUMO: -0.01905 factor:1 | -1 (0.49797) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31671 HOMO: -6.77836 LUMO: -0.82995 factor:1 | -1 (0.54240) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30262 HOMO: -6.48447 LUMO: -0.95512 factor:1 | -1 (0.55650) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40945 HOMO: -7.81239 LUMO: 1.22179 factor:1 | -1 (0.44967) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17018 HOMO: -7.36612 LUMO: 0.19320 factor:1 | -1 (0.68894) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.85122 HOMO: -7.24095 LUMO: 0.33470 factor:1 | 1 (-0.99210) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.16431 HOMO: -7.15932 LUMO: -2.24222 factor:1 | 1 (-1.30519) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.62114 HOMO: -6.88992 LUMO: -2.69937 factor:1 | 1 (-0.76203) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.94599 HOMO: -6.97428 LUMO: -0.98233 factor:1 | 1 (-1.08688) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.17431 HOMO: -7.17564 LUMO: -0.93879 factor:1 | 1 (-0.31519) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.81530 HOMO: -6.81645 LUMO: -1.14288 factor:1 | 1 (-0.95618) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52131 HOMO: -6.83006 LUMO: -0.63403 factor:1 | 1 (-0.66219) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76513 HOMO: -7.17292 LUMO: -1.07213 factor:1 | -1 (0.09399) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.22299 HOMO: -7.53755 LUMO: 0.15510 factor:1 | 1 (-0.36387) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.85802 HOMO: -6.50080 LUMO: -0.51702 factor:1 | 1 (-0.99890) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68275 HOMO: -6.72665 LUMO: -0.80001 factor:1 | 1 (-0.82363) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94641 HOMO: -6.72665 LUMO: 1.68711 factor:1 | 1 (-0.08729) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53161 HOMO: -7.11850 LUMO: -0.75103 factor:1 | -1 (1.32751) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94811 HOMO: -6.87087 LUMO: -0.85988 factor:1 | -1 (0.91101) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.75099 HOMO: -7.08857 LUMO: -0.89798 factor:1 | -1 (1.10813) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88724 HOMO: -6.71305 LUMO: -0.85444 factor:1 | -1 (0.97188) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91850 HOMO: -6.59332 LUMO: -0.60137 factor:1 | -1 (0.94062) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78230 HOMO: -7.28993 LUMO: 0.03265 factor:1 | -1 (0.07682) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47867 HOMO: -7.32258 LUMO: 0.13878 factor:1 | -1 (0.38044) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47038 HOMO: -7.28993 LUMO: 0.11429 factor:1 | -1 (0.38874) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90641 HOMO: -6.86271 LUMO: -1.03947 factor:1 | 1 (-0.04729) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.66709 HOMO: -6.55794 LUMO: -0.84900 factor:1 | -1 (0.19203) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61171 HOMO: -7.03686 LUMO: 0.11429 factor:1 | -1 (0.24741) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79452 HOMO: -7.06952 LUMO: -0.96056 factor:1 | -1 (0.06460) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.61153 HOMO: -6.90897 LUMO: -0.99866 factor:1 | -1 (1.24759) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.67482 HOMO: -7.00693 LUMO: -0.83539 factor:1 | -1 (1.18429) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85953 HOMO: -6.74298 LUMO: -0.85172 factor:1 | -1 (0.99958) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01194 HOMO: -6.83822 LUMO: -1.07213 factor:1 | -1 (0.84717) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91330 HOMO: -7.21918 LUMO: -1.55377 factor:1 | -1 (0.94581) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65793 HOMO: -6.84094 LUMO: -1.09934 factor:1 | 1 (-0.79882) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.59562 HOMO: -7.09129 LUMO: -0.85988 factor:1 | 1 (-0.73650) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03224 HOMO: -6.57971 LUMO: -2.27215 factor:1 | 1 (-0.17312) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.41910 HOMO: -6.81373 LUMO: -1.86942 factor:1 | 1 (-0.55998) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70148 HOMO: -6.59060 LUMO: -2.30480 factor:1 | -1 (0.15764) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79781 HOMO: -6.72938 LUMO: -1.23540 factor:1 | -1 (0.06131) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94813 HOMO: -6.94707 LUMO: -2.62318 factor:1 | 1 (-0.08901) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.81092 HOMO: -7.28177 LUMO: -0.09796 factor:1 | 1 (-0.95180) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06168 HOMO: -6.80013 LUMO: -0.79729 factor:1 | 1 (-0.20256) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14097 HOMO: -7.26544 LUMO: 0.12789 factor:1 | 1 (-0.28186) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10179 HOMO: -6.51713 LUMO: -0.49253 factor:1 | 1 (-0.24267) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17042 HOMO: -6.68856 LUMO: -0.77280 factor:1 | -1 (0.68869) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13732 HOMO: -6.41100 LUMO: -0.70750 factor:1 | -1 (1.72180) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.50277 HOMO: -7.56204 LUMO: 0.22041 factor:1 | -1 (1.35635) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52027 HOMO: -6.68312 LUMO: 1.30343 factor:1 | 1 (-0.66116) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15556 HOMO: -7.24367 LUMO: 0.17415 factor:1 | 1 (-0.29644) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.35782 HOMO: -7.52395 LUMO: 1.16737 factor:1 | 1 (-0.49870) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.02450 HOMO: -6.89264 LUMO: 0.23130 factor:1 | 1 (-1.16538) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.15536 HOMO: -7.21102 LUMO: 0.19048 factor:1 | 1 (-1.29624) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.31681 HOMO: -7.08312 LUMO: 0.25034 factor:1 | 1 (-0.45770) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37877 HOMO: -6.49536 LUMO: -0.65852 factor:1 | 1 (-0.51966) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.07528 HOMO: -6.85455 LUMO: 0.13606 factor:1 | 1 (-1.21616) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.98181 HOMO: -7.10217 LUMO: 0.35919 factor:1 | 1 (-0.12270) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45835 HOMO: -7.77429 LUMO: 1.19186 factor:1 | -1 (0.40077) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15839 HOMO: -6.57427 LUMO: -0.50069 factor:1 | 1 (-0.29927) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27725 HOMO: -7.36340 LUMO: 0.10068 factor:1 | 1 (-0.41813) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08313 HOMO: -7.28177 LUMO: 0.15238 factor:1 | -1 (0.77599) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14830 HOMO: -6.86543 LUMO: -0.84355 factor:1 | -1 (0.71082) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.52787 HOMO: -6.55794 LUMO: 1.39594 factor:1 | -1 (0.33124) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39146 HOMO: -6.26134 LUMO: 1.53744 factor:1 | -1 (0.46765) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.34571 HOMO: -5.97562 LUMO: 1.42316 factor:1 | 1 (-0.48659) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.16693 HOMO: -6.65046 LUMO: 1.44492 factor:1 | 1 (-0.30782) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.21494 HOMO: -6.92258 LUMO: 0.17415 factor:1 | -1 (0.64418) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09570 HOMO: -7.40966 LUMO: 0.19592 factor:1 | -1 (0.76342) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59313 HOMO: -7.17564 LUMO: 0.16871 factor:1 | -1 (0.26599) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99498 HOMO: -7.46953 LUMO: 0.22313 factor:1 | 1 (-0.13587) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.00913 HOMO: -6.13345 LUMO: 1.85854 factor:1 | 1 (-0.15002) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96471 HOMO: -6.99333 LUMO: -1.65717 factor:1 | -1 (0.89441) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94299 HOMO: -6.93074 LUMO: -1.79323 factor:1 | -1 (0.91613) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22400 HOMO: -6.87904 LUMO: -1.79323 factor:1 | -1 (0.63511) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.21015 HOMO: -6.84094 LUMO: 0.66940 factor:1 | -1 (0.64896) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.64408 HOMO: -7.13210 LUMO: -1.17553 factor:1 | 1 (-0.78497) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.37887 HOMO: -6.52801 LUMO: -2.23678 factor:1 | 1 (-1.51976) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.28065 HOMO: -6.81917 LUMO: -1.86398 factor:1 | 1 (-0.42153) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07556 HOMO: -7.30626 LUMO: -1.66806 factor:1 | 1 (-0.21644) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95107 HOMO: -6.98516 LUMO: -1.40683 factor:1 | -1 (0.90804) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58526 HOMO: -6.95523 LUMO: -0.97145 factor:1 | -1 (0.27386) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30224 HOMO: -6.83278 LUMO: -2.68848 factor:1 | -1 (0.55688) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97409 HOMO: -7.25456 LUMO: -2.97420 factor:1 | 1 (-0.11497) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.82273 HOMO: -6.80557 LUMO: -2.65039 factor:1 | 1 (-0.96361) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.02009 HOMO: -7.10489 LUMO: 0.77008 factor:1 | 1 (-1.16097) | 1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.11304 HOMO: -7.28993 LUMO: -1.06124 factor:1 | 1 (-1.25393) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06726 HOMO: -7.11578 LUMO: -1.10206 factor:1 | 1 (-0.20814) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33668 HOMO: -6.91713 LUMO: -1.36329 factor:1 | 1 (-0.47756) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02990 HOMO: -7.07224 LUMO: 0.51974 factor:1 | 1 (-0.17078) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25020 HOMO: -7.22734 LUMO: -0.93335 factor:1 | 1 (-0.39108) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88233 HOMO: -7.19469 LUMO: -0.96600 factor:1 | 1 (-0.02321) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80674 HOMO: -6.93890 LUMO: -0.66940 factor:1 | -1 (0.05238) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.04570 HOMO: -7.09673 LUMO: -1.05852 factor:1 | -1 (1.81342) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.18121 HOMO: -7.19197 LUMO: -2.26943 factor:1 | -1 (1.67791) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.05454 HOMO: -6.90081 LUMO: -2.64767 factor:1 | -1 (1.80458) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30140 HOMO: -6.93890 LUMO: -2.65039 factor:1 | -1 (1.55772) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03896 HOMO: -6.80013 LUMO: -2.54154 factor:1 | 1 (-0.17984) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23322 HOMO: -6.68040 LUMO: -0.89798 factor:1 | 1 (-0.37410) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92611 HOMO: -7.01782 LUMO: -1.09662 factor:1 | 1 (-0.06699) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88059 HOMO: -6.58516 LUMO: -0.83539 factor:1 | 1 (-0.02147) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.01141 HOMO: -7.46953 LUMO: 0.06259 factor:1 | -1 (1.84771) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15441 HOMO: -6.96884 LUMO: -0.99866 factor:1 | -1 (1.70471) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27186 HOMO: -7.29809 LUMO: -0.19320 factor:1 | 1 (-0.41274) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.21145 HOMO: -6.86271 LUMO: 0.04082 factor:1 | 1 (-0.35233) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11469 HOMO: -6.36746 LUMO: -1.02587 factor:1 | 1 (-0.25557) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83855 HOMO: -7.15659 LUMO: -1.25989 factor:1 | -1 (1.02056) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.70889 HOMO: -6.69128 LUMO: -0.59865 factor:1 | -1 (1.15023) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89654 HOMO: -7.09129 LUMO: -1.08573 factor:1 | -1 (0.96258) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.57785 HOMO: -6.64502 LUMO: -0.66396 factor:1 | 1 (-0.71873) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90206 HOMO: -6.93346 LUMO: -0.87349 factor:1 | 1 (-0.04294) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75936 HOMO: -6.77019 LUMO: -0.87349 factor:1 | -1 (0.09976) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89466 HOMO: -6.59060 LUMO: -0.82995 factor:1 | 1 (-0.03554) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.10557 HOMO: -7.17564 LUMO: -1.08846 factor:1 | -1 (2.75355) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.36568 HOMO: -7.27088 LUMO: -1.18642 factor:1 | -1 (2.49343) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.64373 HOMO: -7.06680 LUMO: -1.13199 factor:1 | -1 (2.21539) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.79271 HOMO: -7.21918 LUMO: -1.03947 factor:1 | -1 (2.06641) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.46887 HOMO: -7.26000 LUMO: -0.11973 factor:1 | 1 (-0.60975) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25186 HOMO: -6.77564 LUMO: 0.23402 factor:1 | 1 (-0.39274) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.49655 HOMO: -7.07224 LUMO: -0.75648 factor:1 | -1 (0.36256) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72434 HOMO: -7.45048 LUMO: 0.18232 factor:1 | -1 (0.13478) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17061 HOMO: -7.48313 LUMO: 0.15238 factor:1 | -1 (0.68850) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99692 HOMO: -6.60692 LUMO: -0.50885 factor:1 | -1 (0.86219) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05535 HOMO: -6.62869 LUMO: -0.60954 factor:1 | -1 (0.80377) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18830 HOMO: -7.40422 LUMO: -1.28982 factor:1 | -1 (0.67082) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.99957 HOMO: -6.75114 LUMO: -1.23268 factor:1 | -1 (1.85954) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26975 HOMO: -6.84638 LUMO: -0.73199 factor:1 | -1 (1.58936) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23088 HOMO: -6.79196 LUMO: -1.43676 factor:1 | 1 (-0.37176) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46009 HOMO: -7.00965 LUMO: -1.37690 factor:1 | -1 (0.39903) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33630 HOMO: -6.97972 LUMO: -1.58098 factor:1 | 1 (-0.47718) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18535 HOMO: -6.91169 LUMO: -1.48574 factor:1 | 1 (-0.32624) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.00753 HOMO: -6.90081 LUMO: -1.30343 factor:1 | 1 (-0.14841) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23905 HOMO: -6.78652 LUMO: -1.51840 factor:1 | -1 (0.62007) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.37549 HOMO: -6.84638 LUMO: -1.15104 factor:1 | -1 (0.48363) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57008 HOMO: -6.61237 LUMO: -0.89798 factor:1 | -1 (0.28904) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42923 HOMO: -7.16204 LUMO: -1.30070 factor:1 | -1 (0.42989) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17105 HOMO: -7.32803 LUMO: 0.14694 factor:1 | -1 (0.68807) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.83919 HOMO: -6.99877 LUMO: -0.87621 factor:1 | -1 (2.01993) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.02872 HOMO: -6.99877 LUMO: -0.97145 factor:1 | -1 (1.83040) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31766 HOMO: -7.08040 LUMO: -1.09662 factor:1 | -1 (0.54145) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14944 HOMO: -6.90897 LUMO: -1.14016 factor:1 | -1 (0.70967) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03649 HOMO: -6.68312 LUMO: -0.74831 factor:1 | -1 (0.82263) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99426 HOMO: -6.99061 LUMO: -0.86804 factor:1 | -1 (0.86486) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.20757 HOMO: -7.10761 LUMO: -1.18642 factor:1 | -1 (0.65155) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45184 HOMO: -6.79196 LUMO: -0.71294 factor:1 | -1 (0.40727) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86383 HOMO: -6.86271 LUMO: -0.81362 factor:1 | -1 (0.99528) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62641 HOMO: -7.01510 LUMO: -0.99322 factor:1 | -1 (0.23271) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04136 HOMO: -6.88720 LUMO: -0.87893 factor:1 | -1 (0.81776) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89396 HOMO: -6.88448 LUMO: 0.22041 factor:1 | -1 (0.96516) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87956 HOMO: -7.55932 LUMO: 1.12111 factor:1 | -1 (0.97956) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74685 HOMO: -6.46815 LUMO: -0.86260 factor:1 | -1 (1.11227) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11048 HOMO: -7.13755 LUMO: 0.23130 factor:1 | -1 (0.74864) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92008 HOMO: -6.78924 LUMO: 1.51023 factor:1 | -1 (0.93904) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.29246 HOMO: -6.48992 LUMO: 1.74969 factor:1 | -1 (2.56666) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.59088 HOMO: -6.78380 LUMO: 1.81500 factor:1 | -1 (2.26823) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.75350 HOMO: -6.49536 LUMO: 1.70615 factor:1 | -1 (2.10562) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.05816 HOMO: -6.38651 LUMO: 1.44492 factor:1 | -1 (1.80096) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.08387 HOMO: -6.83822 LUMO: 1.38234 factor:1 | -1 (1.77524) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34791 HOMO: -6.01644 LUMO: 1.20274 factor:1 | -1 (1.51121) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09821 HOMO: -6.18243 LUMO: 1.77962 factor:1 | -1 (1.76090) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37014 HOMO: -6.81917 LUMO: -1.01771 factor:1 | -1 (1.48898) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44614 HOMO: -6.61237 LUMO: -0.91702 factor:1 | -1 (1.41298) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.67820 HOMO: -6.84094 LUMO: -0.84900 factor:1 | -1 (1.18092) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.69325 HOMO: -6.81917 LUMO: -1.01771 factor:1 | -1 (1.16587) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92819 HOMO: -7.86953 LUMO: 1.16737 factor:1 | -1 (0.93093) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.80697 HOMO: -7.40694 LUMO: 0.11429 factor:1 | -1 (2.05215) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.70365 HOMO: -6.70489 LUMO: -0.65035 factor:1 | -1 (2.15547) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.75872 HOMO: -7.23279 LUMO: 0.33470 factor:1 | -1 (2.10039) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91021 HOMO: -7.17020 LUMO: 0.41361 factor:1 | -1 (1.94891) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.02940 HOMO: -6.90353 LUMO: -0.90070 factor:1 | -1 (1.82972) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.89122 HOMO: -7.39061 LUMO: 0.17687 factor:1 | -1 (1.96790) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12426 HOMO: -7.16748 LUMO: 0.42178 factor:1 | -1 (1.73486) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97352 HOMO: -7.36884 LUMO: -1.11295 factor:1 | -1 (0.88559) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86049 HOMO: -7.33347 LUMO: 0.33198 factor:1 | -1 (0.99863) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10727 HOMO: -7.31986 LUMO: -0.83539 factor:1 | -1 (0.75185) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37491 HOMO: -7.31170 LUMO: 0.08708 factor:1 | 1 (-0.51579) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27629 HOMO: -7.36884 LUMO: 0.38096 factor:1 | 1 (-0.41718) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42344 HOMO: -6.99333 LUMO: 1.74153 factor:1 | -1 (0.43568) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.08786 HOMO: -6.94435 LUMO: 1.74969 factor:1 | 1 (-0.22874) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24036 HOMO: -7.02598 LUMO: 1.43404 factor:1 | -1 (0.61876) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50534 HOMO: -6.41100 LUMO: 1.62996 factor:1 | -1 (0.35378) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.14429 HOMO: -6.57699 LUMO: 1.81228 factor:1 | -1 (2.71483) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.01264 HOMO: -6.86543 LUMO: 1.49935 factor:1 | -1 (2.84647) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.21159 HOMO: -6.91169 LUMO: -1.22451 factor:1 | -1 (2.64753) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13277 HOMO: -7.09945 LUMO: -1.23812 factor:1 | -1 (1.72634) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.95255 HOMO: -7.48857 LUMO: 0.10340 factor:1 | -1 (1.90657) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16126 HOMO: -7.21918 LUMO: -0.06803 factor:1 | -1 (1.69785) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.80066 HOMO: -6.34025 LUMO: -0.68845 factor:1 | -1 (2.05846) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.61755 HOMO: -6.82734 LUMO: -0.77825 factor:1 | -1 (2.24157) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.84907 HOMO: -6.92258 LUMO: -1.03675 factor:1 | -1 (2.01005) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39076 HOMO: -6.42461 LUMO: -0.95240 factor:1 | -1 (1.46835) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32137 HOMO: -6.96067 LUMO: -1.05036 factor:1 | -1 (1.53774) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55460 HOMO: -7.23551 LUMO: 0.12245 factor:1 | -1 (1.30451) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.36911 HOMO: -6.85183 LUMO: 0.16055 factor:1 | 1 (-0.51000) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.38422 HOMO: -6.46815 LUMO: -0.89253 factor:1 | 1 (-0.52510) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45623 HOMO: -7.23823 LUMO: -0.06259 factor:1 | -1 (0.40289) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27794 HOMO: -6.76475 LUMO: -0.99049 factor:1 | -1 (0.58118) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.09567 HOMO: -7.14843 LUMO: -0.88165 factor:1 | 1 (-0.23655) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45756 HOMO: -7.15659 LUMO: 0.20681 factor:1 | -1 (0.40156) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53059 HOMO: -7.11306 LUMO: 0.14150 factor:1 | -1 (0.32852) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38134 HOMO: -6.67223 LUMO: -0.86260 factor:1 | -1 (0.47778) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28365 HOMO: -6.92530 LUMO: 0.30749 factor:1 | -1 (0.57547) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25554 HOMO: -6.50624 LUMO: -0.70477 factor:1 | -1 (0.60358) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50651 HOMO: -7.35524 LUMO: 0.75103 factor:1 | -1 (0.35261) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90781 HOMO: -7.07768 LUMO: -0.26939 factor:1 | -1 (0.95131) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15015 HOMO: -7.15932 LUMO: 0.42450 factor:1 | -1 (0.70897) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33560 HOMO: -7.46136 LUMO: 0.04626 factor:1 | -1 (0.52352) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22896 HOMO: -7.05047 LUMO: -1.06669 factor:1 | -1 (0.63016) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03801 HOMO: -6.66951 LUMO: -0.99322 factor:1 | -1 (0.82110) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05872 HOMO: -7.01782 LUMO: -1.08846 factor:1 | -1 (0.80040) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27976 HOMO: -7.03959 LUMO: -1.15376 factor:1 | -1 (0.57936) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.86379 HOMO: -6.68856 LUMO: 1.61364 factor:1 | -1 (1.99533) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.14265 HOMO: -6.53345 LUMO: 1.60275 factor:1 | -1 (1.71647) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38501 HOMO: -6.73482 LUMO: 1.86398 factor:1 | -1 (0.47410) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10787 HOMO: -6.87632 LUMO: 1.59731 factor:1 | -1 (0.75125) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.81818 HOMO: -6.31848 LUMO: 2.12521 factor:1 | -1 (2.04094) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.07549 HOMO: -6.35114 LUMO: 1.71432 factor:1 | -1 (1.78362) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40327 HOMO: -6.34842 LUMO: 1.92929 factor:1 | -1 (0.45585) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32507 HOMO: -6.14977 LUMO: 1.78235 factor:1 | -1 (0.53405) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.81493 HOMO: -6.31032 LUMO: 1.51567 factor:1 | -1 (1.04418) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53266 HOMO: -6.25862 LUMO: 1.75241 factor:1 | -1 (0.32645) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08729 HOMO: -6.49264 LUMO: 1.66806 factor:1 | -1 (0.77182) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.66033 HOMO: -6.28311 LUMO: 1.60003 factor:1 | -1 (2.19879) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91783 HOMO: -7.13210 LUMO: -0.04354 factor:1 | -1 (1.94129) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.73048 HOMO: -7.35252 LUMO: 0.03537 factor:1 | -1 (2.12864) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.97043 HOMO: -6.58243 LUMO: -0.48980 factor:1 | -1 (1.88869) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46992 HOMO: -6.90081 LUMO: -0.05442 factor:1 | -1 (1.38920) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.75706 HOMO: -7.22734 LUMO: 0.17143 factor:1 | -1 (1.10206) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.84675 HOMO: -7.13210 LUMO: -0.99866 factor:1 | -1 (2.01236) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10099 HOMO: -7.39878 LUMO: 0.13334 factor:1 | -1 (1.75813) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.34127 HOMO: -7.04503 LUMO: -0.89798 factor:1 | 1 (-1.48215) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.98145 HOMO: -6.95523 LUMO: -1.07213 factor:1 | 1 (-1.12233) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.31891 HOMO: -6.75114 LUMO: -1.28438 factor:1 | 1 (-0.45979) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.14771 HOMO: -6.75114 LUMO: -0.11701 factor:1 | 1 (-1.28860) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.76460 HOMO: -6.83278 LUMO: -0.01633 factor:1 | 1 (-0.90549) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81716 HOMO: -6.93890 LUMO: -0.88981 factor:1 | -1 (0.04196) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68678 HOMO: -7.07224 LUMO: -1.08573 factor:1 | 1 (-0.82766) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.61774 HOMO: -6.99877 LUMO: -0.95240 factor:1 | 1 (-0.75863) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02971 HOMO: -7.09129 LUMO: 0.35375 factor:1 | 1 (-0.17059) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.90327 HOMO: -7.09401 LUMO: 0.04354 factor:1 | 1 (-1.04416) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.77100 HOMO: -6.85183 LUMO: -0.68573 factor:1 | 1 (-0.91188) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.88629 HOMO: -6.83006 LUMO: -0.58777 factor:1 | -1 (1.97283) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13128 HOMO: -7.40422 LUMO: 0.17687 factor:1 | -1 (1.72784) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98792 HOMO: -7.15932 LUMO: 0.10340 factor:1 | -1 (0.87120) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78190 HOMO: -7.03414 LUMO: -0.19592 factor:1 | -1 (1.07722) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.75093 HOMO: -6.48447 LUMO: -0.36191 factor:1 | -1 (1.10818) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88136 HOMO: -7.49402 LUMO: 0.11429 factor:1 | -1 (0.97776) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01156 HOMO: -7.01237 LUMO: -1.06397 factor:1 | -1 (0.84755) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94299 HOMO: -6.67223 LUMO: -1.07213 factor:1 | -1 (0.91613) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.67063 HOMO: -7.38789 LUMO: -1.15376 factor:1 | -1 (1.18848) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89306 HOMO: -6.42461 LUMO: -1.23812 factor:1 | -1 (0.96606) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.84828 HOMO: -7.36884 LUMO: -1.19186 factor:1 | 1 (-0.98916) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68161 HOMO: -6.65591 LUMO: 0.07075 factor:1 | 1 (-0.82249) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79746 HOMO: -7.39061 LUMO: -0.16871 factor:1 | -1 (0.06166) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15145 HOMO: -6.90353 LUMO: -0.96056 factor:1 | 1 (-0.29233) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52256 HOMO: -7.42054 LUMO: 0.19048 factor:1 | 1 (-0.66344) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76129 HOMO: -7.40150 LUMO: 0.35647 factor:1 | -1 (0.09782) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.77384 HOMO: -6.56067 LUMO: -0.96056 factor:1 | -1 (0.08528) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.81040 HOMO: -6.89809 LUMO: -0.81090 factor:1 | 1 (-0.95128) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94413 HOMO: -6.91986 LUMO: -0.84900 factor:1 | 1 (-0.08501) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03934 HOMO: -6.61509 LUMO: -0.62042 factor:1 | 1 (-0.18022) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.51037 HOMO: -6.58243 LUMO: -0.65579 factor:1 | 1 (-0.65125) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.12788 HOMO: -6.52257 LUMO: -0.92519 factor:1 | 1 (-1.26876) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.28857 HOMO: -6.69128 LUMO: 1.49118 factor:1 | 1 (-0.42945) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30386 HOMO: -7.02870 LUMO: 1.67894 factor:1 | 1 (-0.44474) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96102 HOMO: -6.88720 LUMO: 1.68711 factor:1 | 1 (-0.10191) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00833 HOMO: -5.89943 LUMO: 1.03675 factor:1 | -1 (0.85079) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97325 HOMO: -6.40556 LUMO: 1.14560 factor:1 | -1 (0.88587) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24030 HOMO: -6.51168 LUMO: 1.48030 factor:1 | -1 (0.61881) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18701 HOMO: -6.64502 LUMO: 1.91568 factor:1 | 1 (-0.32790) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.05171 HOMO: -6.47903 LUMO: 1.91296 factor:1 | 1 (-1.19259) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99575 HOMO: -6.34297 LUMO: 1.91840 factor:1 | 1 (-0.13663) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07961 HOMO: -6.89809 LUMO: 1.82861 factor:1 | 1 (-0.22049) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27502 HOMO: -6.10079 LUMO: 1.62996 factor:1 | 1 (-0.41590) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.82293 HOMO: -7.16476 LUMO: -0.92247 factor:1 | -1 (0.03619) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90540 HOMO: -7.10489 LUMO: -0.95784 factor:1 | 1 (-0.04629) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65819 HOMO: -6.76475 LUMO: -0.99866 factor:1 | -1 (0.20093) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93803 HOMO: -6.81373 LUMO: -1.05036 factor:1 | 1 (-0.07891) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.94670 HOMO: -6.90081 LUMO: -1.03947 factor:1 | -1 (1.91242) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98092 HOMO: -7.06952 LUMO: -0.91702 factor:1 | -1 (0.87819) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92179 HOMO: -6.73482 LUMO: -0.94151 factor:1 | -1 (0.93732) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12169 HOMO: -6.99605 LUMO: -1.04764 factor:1 | -1 (0.73743) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09069 HOMO: -7.03686 LUMO: -0.93335 factor:1 | -1 (0.76842) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.69178 HOMO: -6.81101 LUMO: -0.95240 factor:1 | -1 (2.16733) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.09286 HOMO: -6.83822 LUMO: -0.65307 factor:1 | -1 (2.76626) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.62977 HOMO: -7.05319 LUMO: -0.81634 factor:1 | -1 (2.22935) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24198 HOMO: -7.57565 LUMO: 0.19048 factor:1 | 1 (-0.38286) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14054 HOMO: -6.56067 LUMO: -0.50613 factor:1 | 1 (-0.28142) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.34397 HOMO: -6.74298 LUMO: -0.70477 factor:1 | 1 (-0.48485) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41889 HOMO: -7.02054 LUMO: 0.03537 factor:1 | -1 (0.44023) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94424 HOMO: -7.33347 LUMO: -0.17960 factor:1 | -1 (0.91487) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86000 HOMO: -6.98244 LUMO: -0.88165 factor:1 | -1 (0.99912) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07510 HOMO: -7.14843 LUMO: -1.19730 factor:1 | -1 (0.78401) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02215 HOMO: -7.17564 LUMO: -1.21907 factor:1 | -1 (0.83697) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.88988 HOMO: -6.74026 LUMO: -0.86532 factor:1 | -1 (1.96923) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05395 HOMO: -6.82462 LUMO: -1.24084 factor:1 | 1 (-0.19483) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14029 HOMO: -6.78924 LUMO: -0.70477 factor:1 | 1 (-0.28118) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19355 HOMO: -7.41238 LUMO: 0.05987 factor:1 | -1 (0.66556) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99779 HOMO: -6.75931 LUMO: 0.02721 factor:1 | 1 (-0.13867) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11897 HOMO: -6.28583 LUMO: -0.93063 factor:1 | -1 (0.74015) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18685 HOMO: -6.69128 LUMO: -0.83539 factor:1 | 1 (-0.32773) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31968 HOMO: -7.22190 LUMO: 0.01361 factor:1 | -1 (0.53944) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33777 HOMO: -6.95251 LUMO: -1.09934 factor:1 | -1 (0.52134) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41903 HOMO: -6.75387 LUMO: -0.90614 factor:1 | -1 (0.44009) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09549 HOMO: -7.48585 LUMO: 0.05987 factor:1 | -1 (1.76362) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.74199 HOMO: -6.92802 LUMO: -0.66940 factor:1 | 1 (-0.88287) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.86366 HOMO: -7.29537 LUMO: -0.14150 factor:1 | 1 (-0.00454) | 1 | 1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.04625 HOMO: -6.57155 LUMO: -0.86804 factor:1 | 1 (-0.18713) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90731 HOMO: -6.87632 LUMO: -0.77825 factor:1 | 1 (-0.04819) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10924 HOMO: -6.45998 LUMO: -0.31565 factor:1 | 1 (-0.25013) | -1 | -1 |
| G: -6258.49342 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.01285 HOMO: -7.51306 LUMO: 0.05714 factor:1 | -1 (1.84627) | 1 | 1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83319 HOMO: -6.86271 LUMO: -0.00816 factor:1 | 1 (-0.05029) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90577 HOMO: -6.43277 LUMO: -1.07485 factor:1 | 1 (-0.12286) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.81143 HOMO: -6.78108 LUMO: -0.81362 factor:1 | -1 (0.97147) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.76632 HOMO: -6.88448 LUMO: 1.21907 factor:1 | -1 (1.01659) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.79222 HOMO: -6.97700 LUMO: 1.44765 factor:1 | -1 (0.99068) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52764 HOMO: -6.89537 LUMO: 2.12249 factor:1 | -1 (0.25527) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26042 HOMO: -6.28311 LUMO: 1.45037 factor:1 | -1 (0.52249) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79540 HOMO: -6.55522 LUMO: 1.39867 factor:1 | 1 (-0.01249) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37977 HOMO: -6.46815 LUMO: 1.50207 factor:1 | -1 (0.40314) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89148 HOMO: -6.43549 LUMO: 2.17419 factor:1 | 1 (-0.10857) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89268 HOMO: -6.99333 LUMO: 1.87214 factor:1 | 1 (-0.10977) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.73235 HOMO: -6.65591 LUMO: 1.37962 factor:1 | -1 (0.05056) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85232 HOMO: -6.82734 LUMO: 1.55649 factor:1 | 1 (-0.06942) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83923 HOMO: -6.71849 LUMO: 1.36057 factor:1 | 1 (-0.05633) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.54867 HOMO: -6.79468 LUMO: 1.82044 factor:1 | -1 (0.23424) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84936 HOMO: -6.61237 LUMO: 1.15104 factor:1 | 1 (-0.06645) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.63082 HOMO: -6.62053 LUMO: 2.33474 factor:1 | -1 (0.15208) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77570 HOMO: -6.55794 LUMO: 1.65717 factor:1 | -1 (0.00721) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90125 HOMO: -6.85999 LUMO: 2.03813 factor:1 | 1 (-0.11834) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91543 HOMO: -6.45726 LUMO: 1.28438 factor:1 | 1 (-0.13252) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90963 HOMO: -6.23685 LUMO: 1.93201 factor:1 | 1 (-0.12672) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.70187 HOMO: -7.06680 LUMO: 1.86942 factor:1 | -1 (0.08104) | 1 | 1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78941 HOMO: -6.89537 LUMO: 2.17147 factor:1 | 1 (-0.00650) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56812 HOMO: -6.80013 LUMO: 1.78779 factor:1 | 1 (-0.78521) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50893 HOMO: -6.45726 LUMO: 1.58370 factor:1 | 1 (-0.72603) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55459 HOMO: -6.52529 LUMO: 1.71976 factor:1 | 1 (-0.77169) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59323 HOMO: -7.22462 LUMO: -1.18642 factor:1 | 1 (-0.81033) | 1 | 1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44588 HOMO: -7.18381 LUMO: -0.78641 factor:1 | 1 (-0.66298) | 1 | 1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45884 HOMO: -6.93346 LUMO: 1.65717 factor:1 | 1 (-0.67593) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18817 HOMO: -6.41644 LUMO: 1.78235 factor:1 | 1 (-0.40526) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36762 HOMO: -6.59876 LUMO: 1.83677 factor:1 | 1 (-0.58472) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61168 HOMO: -6.35658 LUMO: 1.59731 factor:1 | 1 (-0.82878) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.49402 HOMO: -6.60692 LUMO: 1.66534 factor:1 | 1 (-0.71112) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35258 HOMO: -6.83006 LUMO: 2.11705 factor:1 | 1 (-0.56967) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32752 HOMO: -6.89264 LUMO: 1.30070 factor:1 | 1 (-0.54461) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39737 HOMO: -6.90081 LUMO: 2.05174 factor:1 | 1 (-0.61446) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41280 HOMO: -6.74842 LUMO: 1.96194 factor:1 | 1 (-0.62989) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12716 HOMO: -6.58516 LUMO: 1.30887 factor:1 | 1 (-0.34425) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31497 HOMO: -7.00965 LUMO: 2.08167 factor:1 | 1 (-0.53206) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90392 HOMO: -6.86815 LUMO: 2.29664 factor:1 | 1 (-0.12101) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.67308 HOMO: -6.39740 LUMO: 2.02725 factor:1 | -1 (0.10983) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78808 HOMO: -5.95929 LUMO: 1.62724 factor:1 | 1 (-0.00517) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57552 HOMO: -6.71849 LUMO: 1.34696 factor:1 | 1 (-0.79261) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68622 HOMO: -7.26816 LUMO: 1.74153 factor:1 | 1 (-0.90331) | 1 | 1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.38402 HOMO: -6.90897 LUMO: 1.71432 factor:1 | 1 (-1.60112) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30242 HOMO: -6.70489 LUMO: 1.91568 factor:1 | 1 (-1.51951) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69574 HOMO: -6.83278 LUMO: 1.61908 factor:1 | 1 (-0.91283) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.32936 HOMO: -7.17292 LUMO: 1.95378 factor:1 | 1 (-1.54645) | 1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31957 HOMO: -6.53345 LUMO: 1.74153 factor:1 | 1 (-0.53666) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81588 HOMO: -6.53073 LUMO: 1.51023 factor:1 | 1 (-1.03297) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06478 HOMO: -6.93346 LUMO: 2.22861 factor:1 | 1 (-1.28187) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50357 HOMO: -6.47903 LUMO: 2.05446 factor:1 | 1 (-0.72067) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.73511 HOMO: -6.88992 LUMO: 1.57010 factor:1 | 1 (-1.95220) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69759 HOMO: -6.07358 LUMO: 1.95922 factor:1 | 1 (-0.91468) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50123 HOMO: -6.75114 LUMO: 2.18780 factor:1 | 1 (-0.71833) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.63628 HOMO: -6.96339 LUMO: 1.70071 factor:1 | 1 (-0.85338) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47897 HOMO: -7.14843 LUMO: 1.82588 factor:1 | 1 (-0.69607) | 1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35878 HOMO: -6.96339 LUMO: 2.29392 factor:1 | 1 (-0.57587) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65881 HOMO: -6.81645 LUMO: 2.39732 factor:1 | 1 (-0.87591) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91561 HOMO: -6.48447 LUMO: 1.24084 factor:1 | 1 (-1.13270) | -1 | -1 |
| G: -6257.41721 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69462 HOMO: -7.14843 LUMO: 2.01092 factor:1 | 1 (-0.91172) | 1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78622 HOMO: -7.20013 LUMO: -0.34286 factor:1 | 1 (-1.00331) | 1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99569 HOMO: -6.97700 LUMO: -0.15238 factor:1 | 1 (-1.21278) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.66808 HOMO: -7.07768 LUMO: -0.26123 factor:1 | 1 (-1.88518) | 1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.46773 HOMO: -6.99333 LUMO: -0.41361 factor:1 | 1 (-1.68482) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.50604 HOMO: -6.84638 LUMO: -0.40273 factor:1 | 1 (-1.72313) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81286 HOMO: -6.83822 LUMO: -0.26939 factor:1 | 1 (-1.02995) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92938 HOMO: -6.75931 LUMO: -0.93879 factor:1 | 1 (-1.14647) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93414 HOMO: -6.79468 LUMO: -0.39729 factor:1 | 1 (-1.15123) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53280 HOMO: -6.93890 LUMO: 0.43266 factor:1 | 1 (-0.74989) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39371 HOMO: -7.08040 LUMO: -0.85716 factor:1 | 1 (-1.61081) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27393 HOMO: -6.70216 LUMO: -1.41499 factor:1 | 1 (-1.49102) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.81885 HOMO: -6.63686 LUMO: -0.52790 factor:1 | 1 (-0.03595) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80868 HOMO: -6.75114 LUMO: -0.13334 factor:1 | 1 (-0.02577) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74021 HOMO: -6.94435 LUMO: -0.24490 factor:1 | -1 (0.04269) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69852 HOMO: -6.74298 LUMO: -0.84627 factor:1 | 1 (-0.91561) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50809 HOMO: -7.15932 LUMO: 0.22041 factor:1 | 1 (-0.72518) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79768 HOMO: -6.90081 LUMO: -1.16737 factor:1 | 1 (-0.01478) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.81499 HOMO: -7.04775 LUMO: -0.84355 factor:1 | 1 (-0.03208) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59473 HOMO: -7.17020 LUMO: -1.31159 factor:1 | 1 (-0.81182) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45378 HOMO: -7.14571 LUMO: -0.46259 factor:1 | 1 (-0.67087) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58011 HOMO: -7.45048 LUMO: -0.91158 factor:1 | 1 (-1.79720) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79966 HOMO: -6.87360 LUMO: -0.82995 factor:1 | 1 (-1.01675) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81185 HOMO: -7.43415 LUMO: -0.65307 factor:1 | 1 (-1.02894) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.70999 HOMO: -7.47225 LUMO: -0.77280 factor:1 | 1 (-1.92708) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.97770 HOMO: -6.86271 LUMO: -0.83811 factor:1 | 1 (-2.19479) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59060 HOMO: -7.53483 LUMO: -0.66124 factor:1 | 1 (-0.80769) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.97187 HOMO: -7.45864 LUMO: -1.08301 factor:1 | 1 (-2.18897) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.61695 HOMO: -7.24639 LUMO: -1.19186 factor:1 | 1 (-1.83405) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84665 HOMO: -7.54844 LUMO: -0.96873 factor:1 | 1 (-1.06375) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24233 HOMO: -7.12666 LUMO: -0.01633 factor:1 | 1 (-1.45943) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.28084 HOMO: -6.77291 LUMO: -0.70477 factor:1 | 1 (-1.49793) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20555 HOMO: -6.76475 LUMO: -1.15921 factor:1 | 1 (-1.42264) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65236 HOMO: -5.37697 LUMO: -0.56600 factor:1 | 1 (-0.86946) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.22304 HOMO: -6.62053 LUMO: -1.75513 factor:1 | 1 (-1.44014) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.98698 HOMO: -6.60420 LUMO: -1.74697 factor:1 | 1 (-1.20408) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11711 HOMO: -6.84366 LUMO: -0.94968 factor:1 | 1 (-1.33420) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.16505 HOMO: -6.96884 LUMO: -2.11977 factor:1 | 1 (-1.38215) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.71489 HOMO: -6.80829 LUMO: 0.56055 factor:1 | 1 (-1.93198) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.16415 HOMO: -7.02326 LUMO: 0.11429 factor:1 | 1 (-2.38124) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62066 HOMO: -7.40966 LUMO: 0.18232 factor:1 | 1 (-0.83776) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.17994 HOMO: -6.34570 LUMO: 0.41089 factor:1 | 1 (-1.39703) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24489 HOMO: -6.78924 LUMO: 0.49525 factor:1 | 1 (-1.46199) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13295 HOMO: -6.87632 LUMO: 0.44082 factor:1 | 1 (-1.35004) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24233 HOMO: -6.69944 LUMO: 1.20546 factor:1 | 1 (-1.45943) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.11865 HOMO: -6.83006 LUMO: 1.28982 factor:1 | 1 (-2.33574) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.84558 HOMO: -7.78246 LUMO: 0.20681 factor:1 | 1 (-2.06268) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25357 HOMO: -6.55794 LUMO: -1.65173 factor:1 | 1 (-1.47067) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25643 HOMO: -6.77564 LUMO: -1.14560 factor:1 | 1 (-1.47352) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05486 HOMO: -7.46680 LUMO: -1.18097 factor:1 | 1 (-0.27195) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13817 HOMO: -6.88176 LUMO: -1.24900 factor:1 | 1 (-1.35526) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03760 HOMO: -7.28177 LUMO: -0.42178 factor:1 | 1 (-1.25469) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.48108 HOMO: -7.71715 LUMO: 0.19592 factor:1 | 1 (-2.69817) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.42903 HOMO: -7.02326 LUMO: -1.40683 factor:1 | 1 (-1.64613) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99322 HOMO: -7.27088 LUMO: -1.07485 factor:1 | 1 (-0.21032) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10179 HOMO: -7.17020 LUMO: -0.49525 factor:1 | 1 (-1.31888) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.97976 HOMO: -7.15932 LUMO: 0.02721 factor:1 | 1 (-2.19686) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20321 HOMO: -7.00693 LUMO: -0.83267 factor:1 | 1 (-1.42030) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07561 HOMO: -6.86543 LUMO: -0.10340 factor:1 | 1 (-1.29270) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.09479 HOMO: -7.11850 LUMO: -0.08980 factor:1 | 1 (-2.31188) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56091 HOMO: -6.87087 LUMO: -0.88981 factor:1 | 1 (-0.77800) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65808 HOMO: -7.08857 LUMO: -1.27077 factor:1 | 1 (-0.87517) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38912 HOMO: -6.79468 LUMO: -0.81906 factor:1 | 1 (-0.60622) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48639 HOMO: -6.86815 LUMO: -0.89798 factor:1 | 1 (-1.70349) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12356 HOMO: -6.78652 LUMO: -2.00548 factor:1 | 1 (-1.34065) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41271 HOMO: -6.75114 LUMO: -0.08436 factor:1 | 1 (-0.62981) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.59293 HOMO: -6.55794 LUMO: 0.52790 factor:1 | 1 (-1.81002) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08286 HOMO: -7.17836 LUMO: 0.28300 factor:1 | 1 (-0.29995) | 1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.51328 HOMO: -7.35796 LUMO: -0.77552 factor:1 | 1 (-1.73037) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60080 HOMO: -7.23551 LUMO: -1.17553 factor:1 | 1 (-0.81789) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.87530 HOMO: -7.07496 LUMO: -1.14288 factor:1 | 1 (-2.09239) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39687 HOMO: -6.70489 LUMO: -0.83539 factor:1 | 1 (-1.61396) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22257 HOMO: -6.59604 LUMO: -0.89798 factor:1 | -1 (0.56034) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22681 HOMO: -6.94162 LUMO: -1.22451 factor:1 | 1 (-0.44390) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36899 HOMO: -6.68040 LUMO: 0.22041 factor:1 | 1 (-0.58608) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14923 HOMO: -6.88176 LUMO: 0.11157 factor:1 | 1 (-0.36632) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08909 HOMO: -6.91713 LUMO: 1.27621 factor:1 | 1 (-0.30618) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23448 HOMO: -6.77836 LUMO: 1.01226 factor:1 | 1 (-0.45157) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62151 HOMO: -7.14571 LUMO: 1.48574 factor:1 | 1 (-0.83860) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26126 HOMO: -6.96884 LUMO: 1.48574 factor:1 | 1 (-0.47835) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.64109 HOMO: -7.24367 LUMO: 1.28438 factor:1 | 1 (-1.85818) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.09920 HOMO: -7.10489 LUMO: 1.29526 factor:1 | 1 (-1.31630) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65916 HOMO: -7.07224 LUMO: 1.29254 factor:1 | 1 (-1.87625) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94339 HOMO: -7.12938 LUMO: 0.49253 factor:1 | 1 (-1.16048) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15041 HOMO: -7.33619 LUMO: 1.45581 factor:1 | 1 (-1.36751) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33624 HOMO: -6.87904 LUMO: -0.14422 factor:1 | 1 (-1.55333) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.47502 HOMO: -6.81917 LUMO: 0.50341 factor:1 | 1 (-1.69211) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56104 HOMO: -7.27905 LUMO: 0.13606 factor:1 | 1 (-0.77814) | 1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72020 HOMO: -6.87904 LUMO: -0.09796 factor:1 | 1 (-0.93730) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78156 HOMO: -7.33891 LUMO: 0.03810 factor:1 | 1 (-0.99866) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57699 HOMO: -6.98516 LUMO: 0.98233 factor:1 | 1 (-0.79408) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38839 HOMO: -6.94162 LUMO: 0.86804 factor:1 | 1 (-0.60548) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39329 HOMO: -7.37701 LUMO: 0.05442 factor:1 | 1 (-0.61038) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.82047 HOMO: -7.04775 LUMO: 0.43266 factor:1 | 1 (-2.03756) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47685 HOMO: -7.47497 LUMO: 0.31837 factor:1 | 1 (-0.69394) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13841 HOMO: -6.62053 LUMO: 0.13061 factor:1 | 1 (-1.35551) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.79826 HOMO: -6.44366 LUMO: -0.04354 factor:1 | 1 (-2.01536) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.98444 HOMO: -6.40284 LUMO: 0.68301 factor:1 | 1 (-2.20154) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.50607 HOMO: -6.73754 LUMO: 0.36735 factor:1 | 1 (-1.72316) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02494 HOMO: -6.85455 LUMO: 0.23946 factor:1 | 1 (-1.24204) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10429 HOMO: -6.93346 LUMO: 0.24762 factor:1 | 1 (-1.32138) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.16081 HOMO: -6.85455 LUMO: 0.17687 factor:1 | 1 (-1.37790) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27447 HOMO: -6.62325 LUMO: 0.69933 factor:1 | 1 (-1.49156) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30965 HOMO: -6.43005 LUMO: 0.50069 factor:1 | -1 (0.47326) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.41328 HOMO: -6.56883 LUMO: 0.22858 factor:1 | 1 (-1.63037) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02000 HOMO: -6.78380 LUMO: 0.54967 factor:1 | 1 (-0.23709) | -1 | -1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52716 HOMO: -7.35524 LUMO: 0.00272 factor:1 | 1 (-1.74425) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02902 HOMO: -7.27360 LUMO: 0.08436 factor:1 | 1 (-1.24612) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.54305 HOMO: -7.44504 LUMO: -0.96056 factor:1 | -1 (1.23986) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91228 HOMO: -7.27360 LUMO: 0.29933 factor:1 | -1 (0.87063) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68272 HOMO: -7.09129 LUMO: 0.41089 factor:1 | 1 (-1.89982) | 1 | 1 |
| G: -6257.41721 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79354 HOMO: -6.93618 LUMO: 0.36463 factor:1 | 1 (-1.01063) | -1 | -1 |
| G: -6257.41721 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31045 HOMO: -7.65728 LUMO: 0.20136 factor:1 | 1 (-0.52755) | 1 | 1 |
| G: -6257.41721 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36956 HOMO: -6.90353 LUMO: -0.92791 factor:1 | 1 (-0.58665) | -1 | -1 |
| G: -6257.41721 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38625 HOMO: -6.82462 LUMO: -1.18370 factor:1 | -1 (0.39666) | -1 | -1 |
| G: -6257.41721 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29485 HOMO: -7.09129 LUMO: -0.13334 factor:1 | 1 (-1.51195) | 1 | 1 |
| G: -6257.41721 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.43872 HOMO: -7.40966 LUMO: -1.06941 factor:1 | 1 (-1.65581) | 1 | 1 |
| G: -6257.41721 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56243 HOMO: -7.24367 LUMO: -1.00954 factor:1 | 1 (-0.77952) | 1 | 1 |
| G: -6257.41721 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74015 HOMO: -7.51851 LUMO: 0.09796 factor:1 | 1 (-0.95724) | 1 | 1 |
| G: -6257.41721 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62464 HOMO: -7.48857 LUMO: -0.07619 factor:1 | 1 (-0.84173) | 1 | 1 |
| G: -6257.41721 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26097 HOMO: -6.53345 LUMO: 1.09390 factor:1 | -1 (0.52194) | -1 | -1 |
| G: -6257.41721 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48463 HOMO: -7.21918 LUMO: 0.08436 factor:1 | 1 (-0.70173) | 1 | 1 |
| G: -6257.41721 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48039 HOMO: -7.38789 LUMO: 1.02587 factor:1 | 1 (-0.69748) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75873 HOMO: -6.83550 LUMO: -0.67484 factor:1 | 1 (-0.97583) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23889 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-0.45598) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.34235 HOMO: -6.79740 LUMO: 1.91296 factor:1 | 1 (-0.55944) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04569 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-0.26278) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.73374 HOMO: -6.62597 LUMO: -0.44082 factor:1 | -1 (1.04916) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.25737 HOMO: -6.45182 LUMO: -0.20409 factor:1 | -1 (0.52553) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45082 HOMO: -6.51168 LUMO: -0.23130 factor:1 | -1 (0.33209) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.54029 HOMO: -7.14027 LUMO: 0.49797 factor:1 | -1 (0.24262) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82952 HOMO: -7.55660 LUMO: 0.24762 factor:1 | 1 (-0.04661) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08544 HOMO: -6.88992 LUMO: -0.64763 factor:1 | 1 (-0.30254) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.04616 HOMO: -6.72665 LUMO: -0.45987 factor:1 | -1 (0.73675) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20540 HOMO: -6.72121 LUMO: -0.58232 factor:1 | -1 (0.57751) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24671 HOMO: -7.26816 LUMO: 0.32926 factor:1 | -1 (0.53620) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23742 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-0.45451) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.56269 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-1.77979) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60192 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-0.81901) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.36313 HOMO: -6.77019 LUMO: -0.62858 factor:1 | -1 (1.41978) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43479 HOMO: -6.82462 LUMO: -0.67484 factor:1 | -1 (0.34812) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.00142 HOMO: -6.79740 LUMO: -0.55511 factor:1 | -1 (0.78148) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.66427 HOMO: -6.79740 LUMO: -0.67756 factor:1 | -1 (0.11864) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.40231 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-1.61940) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47922 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-0.69631) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.50408 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-1.72117) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71642 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-0.93351) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.66023 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-0.87732) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.37511 HOMO: -6.59332 LUMO: -0.27211 factor:1 | 1 (-0.59220) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47870 HOMO: -6.57427 LUMO: -0.16871 factor:1 | 1 (-0.69580) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.43870 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-0.65579) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.25854 HOMO: -6.72121 LUMO: 2.00004 factor:1 | -1 (0.52436) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50145 HOMO: -6.61509 LUMO: 1.55921 factor:1 | 1 (-0.71854) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.18235 HOMO: -6.55250 LUMO: 1.73064 factor:1 | -1 (0.60056) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70423 HOMO: -6.66135 LUMO: 2.02181 factor:1 | 1 (-0.92132) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.20158 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-0.41867) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.03454 HOMO: -6.66679 LUMO: 1.98371 factor:1 | -1 (0.74837) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13179 HOMO: -6.67495 LUMO: 2.04085 factor:1 | -1 (0.65111) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84185 HOMO: -6.89809 LUMO: 1.95106 factor:1 | 1 (-0.05894) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21133 HOMO: -6.50352 LUMO: 1.88847 factor:1 | -1 (0.57158) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.31531 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-2.53240) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.00643 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-2.22352) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29757 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-1.51467) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.14532 HOMO: -6.65591 LUMO: 2.20684 factor:1 | 1 (-2.36241) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.90825 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-2.12535) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30064 HOMO: -6.35114 LUMO: 1.92112 factor:1 | -1 (0.48227) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08240 HOMO: -6.53617 LUMO: 1.75241 factor:1 | 1 (-0.29949) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17622 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-0.39331) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03513 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-0.25222) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.85231 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-2.06940) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.02009 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-2.23718) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12236 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-1.33945) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20231 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-1.41940) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.28105 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-2.49814) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.67486 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-1.89195) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.08282 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-1.29992) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38213 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-0.59922) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.17253 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-2.38962) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.40182 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-1.61891) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92546 HOMO: -6.90897 LUMO: 1.91296 factor:1 | 1 (-1.14255) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15452 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-1.37162) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32553 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-0.54262) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.53766 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-1.75475) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18438 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-0.40148) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.16040 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-1.37749) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.40005 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-1.61715) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55070 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-0.76780) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.77829 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-1.99538) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93286 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-1.14995) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30070 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-1.51780) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.31005 HOMO: -6.51168 LUMO: 2.10072 factor:1 | -1 (0.47285) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26711 HOMO: -7.03686 LUMO: 2.12249 factor:1 | -1 (0.51579) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29242 HOMO: -6.84094 LUMO: 1.63268 factor:1 | -1 (0.49049) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20790 HOMO: -6.75387 LUMO: 1.72248 factor:1 | -1 (0.57500) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24287 HOMO: -6.86271 LUMO: 1.68711 factor:1 | -1 (0.54004) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.06706 HOMO: -6.84094 LUMO: 2.02997 factor:1 | -1 (0.71585) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65471 HOMO: -6.80557 LUMO: 2.02725 factor:1 | 1 (-0.87180) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70173 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-0.91882) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56679 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-0.78388) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42578 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-0.64287) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15988 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-1.37698) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.09997 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-1.31706) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48609 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-1.70319) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.53956 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-1.75666) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06223 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-0.27932) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13649 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-0.35358) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33712 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-0.55421) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24923 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-0.46632) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28477 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-0.50186) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41388 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-0.63098) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46442 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-0.68151) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13486 HOMO: -6.64230 LUMO: 2.16058 factor:1 | 1 (-0.35195) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40681 HOMO: -6.58788 LUMO: 2.10616 factor:1 | 1 (-0.62390) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14359 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-0.36069) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46768 HOMO: -6.31304 LUMO: 2.31841 factor:1 | 1 (-0.68477) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03954 HOMO: -6.94979 LUMO: 2.07895 factor:1 | 1 (-0.25663) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25200 HOMO: -6.88992 LUMO: 2.28031 factor:1 | 1 (-0.46910) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46178 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-0.67887) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23777 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-0.45487) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.49525 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-0.71234) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.34406 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-0.56115) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18727 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-0.40436) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28207 HOMO: -6.31304 LUMO: 2.18507 factor:1 | 1 (-0.49917) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24686 HOMO: -6.18243 LUMO: 2.01636 factor:1 | 1 (-0.46395) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47070 HOMO: -6.99877 LUMO: 2.14970 factor:1 | 1 (-0.68779) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79128 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-1.00837) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90350 HOMO: -6.36202 LUMO: 2.17419 factor:1 | 1 (-1.12059) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99939 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-1.21649) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81604 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-1.03313) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.87456 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-2.09166) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.40500 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-2.62209) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54521 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-0.76230) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14380 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-1.36090) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.17959 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-1.39668) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93278 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-1.14987) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35383 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-0.57092) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32243 HOMO: -6.44094 LUMO: 1.74425 factor:1 | 1 (-0.53952) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53280 HOMO: -6.51985 LUMO: 1.84221 factor:1 | 1 (-0.74989) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.05756 HOMO: -6.63414 LUMO: -0.24762 factor:1 | -1 (0.72535) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88541 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-0.10251) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32635 HOMO: -7.19741 LUMO: 0.58232 factor:1 | 1 (-0.54344) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24403 HOMO: -6.77019 LUMO: -0.56872 factor:1 | 1 (-0.46112) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87997 HOMO: -7.46136 LUMO: 0.28844 factor:1 | 1 (-0.09706) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28175 HOMO: -6.60420 LUMO: -0.54151 factor:1 | 1 (-0.49884) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11674 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-0.33383) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.04018 HOMO: -6.81645 LUMO: -0.57144 factor:1 | 1 (-1.25727) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.16127 HOMO: -7.48041 LUMO: 0.28572 factor:1 | 1 (-1.37837) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.72077 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-1.93786) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81819 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-1.03528) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.82965 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-1.04674) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30278 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-0.51987) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24343 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-0.46053) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78306 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-1.00015) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.86010 HOMO: -6.50896 LUMO: -0.25034 factor:1 | 1 (-1.07719) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23312 HOMO: -7.17564 LUMO: -0.68573 factor:1 | 1 (-0.45021) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14795 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-0.36504) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.77231 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-0.98941) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.66224 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-0.87934) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18928 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-0.40637) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98846 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-0.20555) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.41554 HOMO: -6.62325 LUMO: 2.02725 factor:1 | 1 (-1.63263) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.12137 HOMO: -6.63414 LUMO: 1.91296 factor:1 | 1 (-2.33846) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.18145 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-2.39855) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71144 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-0.92853) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17608 HOMO: -6.61237 LUMO: 2.11432 factor:1 | 1 (-0.39318) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58991 HOMO: -6.62053 LUMO: 2.09256 factor:1 | 1 (-1.80700) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.07348 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-2.29057) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12386 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-1.34095) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86419 HOMO: -6.85183 LUMO: 2.12793 factor:1 | 1 (-0.08128) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18444 HOMO: -6.81101 LUMO: 1.83949 factor:1 | 1 (-0.40153) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92998 HOMO: -6.98788 LUMO: 2.16058 factor:1 | 1 (-0.14708) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.53592 HOMO: -6.62869 LUMO: 2.00820 factor:1 | 1 (-1.75301) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.93919 HOMO: -6.34025 LUMO: 2.25855 factor:1 | 1 (-2.15628) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12407 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-1.34117) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62643 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-0.84353) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82791 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-0.04501) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06577 HOMO: -6.83278 LUMO: 1.53744 factor:1 | 1 (-0.28286) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62962 HOMO: -6.41917 LUMO: 1.82316 factor:1 | 1 (-0.84671) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88644 HOMO: -6.56339 LUMO: 1.63813 factor:1 | 1 (-1.10353) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.72240 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-1.93949) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58506 HOMO: -6.63141 LUMO: 1.92112 factor:1 | 1 (-1.80216) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10503 HOMO: -6.83822 LUMO: 1.88847 factor:1 | 1 (-1.32212) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.55483 HOMO: -6.84638 LUMO: 1.90480 factor:1 | 1 (-1.77192) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.85531 HOMO: -6.82462 LUMO: 1.70888 factor:1 | 1 (-1.07240) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88217 HOMO: -6.82734 LUMO: 2.12521 factor:1 | 1 (-1.09926) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18350 HOMO: -6.94435 LUMO: 1.87214 factor:1 | 1 (-1.40060) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32498 HOMO: -6.98516 LUMO: 2.51433 factor:1 | 1 (-0.54208) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28673 HOMO: -6.74026 LUMO: 2.15514 factor:1 | -1 (0.49617) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52709 HOMO: -6.93618 LUMO: 2.54426 factor:1 | -1 (0.25581) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.63118 HOMO: -6.28583 LUMO: 2.53610 factor:1 | -1 (1.15172) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89485 HOMO: -6.56883 LUMO: 1.94834 factor:1 | 1 (-0.11195) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78612 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-0.00321) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24695 HOMO: -6.19059 LUMO: 1.99732 factor:1 | -1 (0.53596) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45307 HOMO: -6.78108 LUMO: 2.03813 factor:1 | 1 (-0.67016) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65634 HOMO: -6.82189 LUMO: 1.77418 factor:1 | 1 (-0.87343) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08278 HOMO: -6.45454 LUMO: 1.78779 factor:1 | 1 (-0.29987) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96465 HOMO: -6.84366 LUMO: 1.77690 factor:1 | 1 (-0.18174) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97159 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-0.18868) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95023 HOMO: -6.76475 LUMO: 2.40277 factor:1 | 1 (-0.16732) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.59009 HOMO: -6.65863 LUMO: 1.86670 factor:1 | -1 (0.19282) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.69554 HOMO: -6.50080 LUMO: 1.93201 factor:1 | 1 (-1.91263) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87419 HOMO: -6.34842 LUMO: 1.70888 factor:1 | 1 (-1.09129) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80918 HOMO: -6.60692 LUMO: 2.20140 factor:1 | 1 (-1.02628) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71264 HOMO: -6.74026 LUMO: 2.14970 factor:1 | 1 (-0.92973) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03058 HOMO: -6.63686 LUMO: 2.17419 factor:1 | 1 (-1.24767) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43988 HOMO: -6.81917 LUMO: 2.10072 factor:1 | -1 (0.34303) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73931 HOMO: -6.92802 LUMO: 2.04358 factor:1 | 1 (-0.95640) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48597 HOMO: -6.56067 LUMO: -0.47620 factor:1 | 1 (-0.70306) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98628 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-0.20338) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89610 HOMO: -6.78380 LUMO: -0.64763 factor:1 | 1 (-1.11319) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74633 HOMO: -6.51985 LUMO: -0.24490 factor:1 | 1 (-0.96342) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99940 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-0.21649) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57248 HOMO: -7.10489 LUMO: -0.62586 factor:1 | -1 (0.21043) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.56516 HOMO: -7.18108 LUMO: 0.48980 factor:1 | -1 (0.21775) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76350 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-0.98059) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67699 HOMO: -6.70761 LUMO: -0.54423 factor:1 | 1 (-0.89408) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22275 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-0.43984) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65946 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-1.87655) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.04738 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-2.26448) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.16342 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-1.38052) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.90148 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-2.11857) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.00176 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-1.21885) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.17567 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-1.39276) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91833 HOMO: -6.66951 LUMO: -0.40817 factor:1 | 1 (-1.13542) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42191 HOMO: -6.60420 LUMO: -0.19320 factor:1 | 1 (-0.63900) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70951 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-0.92660) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46575 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-0.68284) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39972 HOMO: -7.27088 LUMO: 0.53334 factor:1 | -1 (0.38319) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33942 HOMO: -7.20013 LUMO: 0.59049 factor:1 | -1 (0.44349) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94108 HOMO: -6.60148 LUMO: -0.20953 factor:1 | 1 (-1.15817) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06747 HOMO: -6.69400 LUMO: -0.51974 factor:1 | 1 (-1.28457) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.29334 HOMO: -7.40422 LUMO: -0.98777 factor:1 | 1 (-0.51043) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11418 HOMO: -6.88176 LUMO: -0.71022 factor:1 | 1 (-0.33127) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.87190 HOMO: -6.86271 LUMO: -0.59321 factor:1 | 1 (-2.08899) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.25231 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-2.46941) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.74561 HOMO: -6.71033 LUMO: 1.57010 factor:1 | 1 (-1.96270) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.04194 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-2.25903) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.94232 HOMO: -6.67495 LUMO: 2.03813 factor:1 | 1 (-2.15941) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23186 HOMO: -6.54434 LUMO: 1.83677 factor:1 | 1 (-1.44895) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06327 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-0.28036) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88548 HOMO: -6.76747 LUMO: 1.87759 factor:1 | 1 (-1.10258) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90157 HOMO: -6.58243 LUMO: 1.61364 factor:1 | 1 (-1.11866) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.85052 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-1.06761) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16980 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-0.38689) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.73492 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-1.95201) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.66286 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-1.87995) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10824 HOMO: -6.83278 LUMO: 1.91296 factor:1 | 1 (-1.32533) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.86836 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-2.08545) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13763 HOMO: -6.50080 LUMO: 1.73337 factor:1 | 1 (-1.35472) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14179 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-1.35888) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.27560 HOMO: -6.63686 LUMO: 2.20140 factor:1 | -1 (0.50730) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.27626 HOMO: -6.57427 LUMO: 1.87214 factor:1 | -1 (0.50665) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95837 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-0.17546) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04563 HOMO: -6.63958 LUMO: 2.04902 factor:1 | 1 (-0.26273) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92528 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-0.14237) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04637 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-0.26346) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12026 HOMO: -6.72938 LUMO: 2.28304 factor:1 | -1 (0.66265) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91057 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-1.12767) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.04592 HOMO: -6.95523 LUMO: 2.33474 factor:1 | 1 (-1.26302) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.80289 HOMO: -6.59876 LUMO: 2.30480 factor:1 | 1 (-2.01998) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33151 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-1.54860) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96486 HOMO: -7.06408 LUMO: 1.99187 factor:1 | 1 (-1.18195) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19051 HOMO: -6.95795 LUMO: 1.88847 factor:1 | -1 (0.59239) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.05797 HOMO: -6.85455 LUMO: 1.63813 factor:1 | -1 (0.72494) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88272 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-0.09981) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83033 HOMO: -6.91441 LUMO: 1.68983 factor:1 | 1 (-1.04742) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59762 HOMO: -6.89809 LUMO: 2.23678 factor:1 | 1 (-0.81471) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14974 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-0.36684) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91085 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-1.12794) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86704 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-0.08414) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00095 HOMO: -6.94979 LUMO: 2.28031 factor:1 | 1 (-0.21804) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83235 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-0.04944) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68967 HOMO: -6.87360 LUMO: 2.40277 factor:1 | 1 (-0.90677) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95056 HOMO: -6.92802 LUMO: 1.89663 factor:1 | 1 (-0.16765) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69740 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-0.91449) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97839 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-0.19549) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94206 HOMO: -6.54978 LUMO: 1.93201 factor:1 | 1 (-1.15915) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72603 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-0.94312) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84323 HOMO: -6.55794 LUMO: 1.89663 factor:1 | 1 (-1.06032) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93961 HOMO: -6.07630 LUMO: 1.94289 factor:1 | 1 (-1.15670) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02211 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-1.23921) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07052 HOMO: -6.63958 LUMO: -0.61770 factor:1 | 1 (-1.28762) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15114 HOMO: -6.81101 LUMO: -0.57960 factor:1 | -1 (0.63177) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07850 HOMO: -6.74298 LUMO: -0.57960 factor:1 | 1 (-0.29560) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98552 HOMO: -6.63686 LUMO: -0.42994 factor:1 | 1 (-0.20262) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84100 HOMO: -6.60965 LUMO: -0.41089 factor:1 | 1 (-0.05810) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58737 HOMO: -6.60692 LUMO: -0.80274 factor:1 | -1 (0.19554) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06767 HOMO: -6.58788 LUMO: -0.78097 factor:1 | 1 (-0.28477) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05739 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-0.27448) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04582 HOMO: -6.63141 LUMO: -0.40545 factor:1 | 1 (-0.26292) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92707 HOMO: -6.62053 LUMO: -0.83811 factor:1 | 1 (-0.14417) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90917 HOMO: -6.59604 LUMO: -0.35375 factor:1 | 1 (-0.12626) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.71572 HOMO: -6.34297 LUMO: -0.39729 factor:1 | -1 (0.06718) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91744 HOMO: -6.67223 LUMO: 1.97827 factor:1 | 1 (-0.13453) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83841 HOMO: -6.40012 LUMO: 1.89935 factor:1 | 1 (-1.05550) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76769 HOMO: -6.74842 LUMO: 1.97283 factor:1 | 1 (-0.98478) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84233 HOMO: -6.76747 LUMO: 2.17147 factor:1 | 1 (-1.05942) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54853 HOMO: -6.72121 LUMO: 1.55649 factor:1 | 1 (-0.76562) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87030 HOMO: -6.97700 LUMO: 2.04085 factor:1 | 1 (-1.08739) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74722 HOMO: -7.06680 LUMO: 2.04085 factor:1 | 1 (-0.96432) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68635 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-0.90345) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80924 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-1.02633) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19154 HOMO: -6.72665 LUMO: 2.20140 factor:1 | 1 (-0.40863) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32379 HOMO: -6.77291 LUMO: 2.34562 factor:1 | 1 (-0.54088) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03741 HOMO: -6.73754 LUMO: 2.00276 factor:1 | 1 (-0.25451) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01880 HOMO: -7.04231 LUMO: 1.92112 factor:1 | 1 (-0.23590) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06411 HOMO: -6.83822 LUMO: 1.72248 factor:1 | 1 (-0.28120) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99815 HOMO: -6.57971 LUMO: 2.16603 factor:1 | 1 (-0.21524) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97001 HOMO: -6.80013 LUMO: 1.88575 factor:1 | 1 (-0.18711) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72480 HOMO: -6.93618 LUMO: 2.18235 factor:1 | 1 (-0.94189) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65484 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-0.87193) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96954 HOMO: -7.06952 LUMO: 2.18507 factor:1 | 1 (-1.18663) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55555 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-0.77264) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68989 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-0.90698) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80943 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-1.02652) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.98316 HOMO: -7.17292 LUMO: 1.90752 factor:1 | 1 (-2.20026) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30895 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-1.52604) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52269 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-1.73979) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.98814 HOMO: -6.85727 LUMO: 2.13609 factor:1 | 1 (-2.20524) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.82132 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-1.03841) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.43718 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-0.65427) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57933 HOMO: -6.67223 LUMO: 2.07351 factor:1 | 1 (-0.79642) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67517 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-0.89226) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16823 HOMO: -6.90897 LUMO: 2.28848 factor:1 | -1 (0.61468) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15963 HOMO: -7.04231 LUMO: 1.70071 factor:1 | -1 (0.62328) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74018 HOMO: -6.69944 LUMO: 1.94834 factor:1 | 1 (-0.95727) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.66499 HOMO: -6.56067 LUMO: 2.20956 factor:1 | 1 (-0.88208) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88521 HOMO: -6.65046 LUMO: 2.06807 factor:1 | 1 (-1.10231) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38080 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-0.59789) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33070 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-0.54779) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35263 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-0.56972) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78962 HOMO: -6.85183 LUMO: 2.16058 factor:1 | 1 (-1.00671) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.18573 HOMO: -6.54706 LUMO: 1.92384 factor:1 | -1 (0.59718) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21196 HOMO: -6.84366 LUMO: 2.48984 factor:1 | -1 (0.57095) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37697 HOMO: -6.77291 LUMO: 2.46263 factor:1 | -1 (0.40594) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11138 HOMO: -7.01782 LUMO: 2.31025 factor:1 | 1 (-0.32847) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76690 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-0.98399) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30251 HOMO: -6.64230 LUMO: 1.97283 factor:1 | 1 (-0.51960) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30178 HOMO: -6.47359 LUMO: 2.20412 factor:1 | -1 (0.48112) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30872 HOMO: -6.90625 LUMO: 1.92384 factor:1 | -1 (0.47419) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26336 HOMO: -7.17020 LUMO: 2.06807 factor:1 | -1 (0.51955) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.11650 HOMO: -6.65046 LUMO: 2.20956 factor:1 | -1 (0.66641) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.17032 HOMO: -7.07496 LUMO: 1.82861 factor:1 | -1 (0.61258) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33808 HOMO: -6.83006 LUMO: 2.14970 factor:1 | -1 (0.44482) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88060 HOMO: -6.92802 LUMO: 1.99187 factor:1 | 1 (-0.09769) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86212 HOMO: -6.69672 LUMO: 2.36739 factor:1 | 1 (-0.07921) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79700 HOMO: -7.13755 LUMO: 2.00276 factor:1 | 1 (-0.01410) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37876 HOMO: -6.92530 LUMO: 2.25582 factor:1 | -1 (0.40414) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16809 HOMO: -6.77564 LUMO: 1.97827 factor:1 | -1 (0.61481) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09038 HOMO: -6.87904 LUMO: 1.60003 factor:1 | -1 (0.69253) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.00556 HOMO: -6.62869 LUMO: 1.90480 factor:1 | -1 (0.77735) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45647 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-0.67356) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10231 HOMO: -6.74298 LUMO: 1.47486 factor:1 | 1 (-1.31940) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.06923 HOMO: -6.77019 LUMO: 1.90480 factor:1 | -1 (0.71367) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.89309 HOMO: -6.70489 LUMO: 1.99459 factor:1 | -1 (0.88981) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.66028 HOMO: -6.73482 LUMO: 2.08711 factor:1 | 1 (-0.87738) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84772 HOMO: -6.46543 LUMO: 1.73881 factor:1 | 1 (-0.06482) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05937 HOMO: -6.96067 LUMO: 2.26127 factor:1 | 1 (-0.27647) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.68519 HOMO: -6.67767 LUMO: 2.10616 factor:1 | -1 (0.09772) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78027 HOMO: -6.28855 LUMO: 2.35923 factor:1 | -1 (0.00264) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45406 HOMO: -6.80285 LUMO: 1.62724 factor:1 | -1 (0.32885) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38997 HOMO: -6.85455 LUMO: 2.23133 factor:1 | -1 (0.39293) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.49702 HOMO: -6.51713 LUMO: 2.33474 factor:1 | -1 (0.28588) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43969 HOMO: -6.88176 LUMO: 2.15242 factor:1 | -1 (0.34322) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.50214 HOMO: -6.54434 LUMO: 2.32113 factor:1 | -1 (0.28077) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.59226 HOMO: -6.62597 LUMO: 2.24222 factor:1 | -1 (0.19064) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53915 HOMO: -6.74570 LUMO: 2.19868 factor:1 | -1 (0.24376) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53945 HOMO: -6.62869 LUMO: 1.98915 factor:1 | -1 (0.24346) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.63368 HOMO: -6.64502 LUMO: 2.13881 factor:1 | -1 (0.14923) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62763 HOMO: -6.95795 LUMO: 1.82316 factor:1 | 1 (-0.84472) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70271 HOMO: -6.77291 LUMO: 1.36329 factor:1 | 1 (-0.91980) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73218 HOMO: -6.45726 LUMO: 1.73064 factor:1 | 1 (-0.94927) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54053 HOMO: -6.49264 LUMO: 1.77418 factor:1 | 1 (-0.75762) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14370 HOMO: -6.60420 LUMO: 2.20956 factor:1 | 1 (-0.36080) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22569 HOMO: -6.56067 LUMO: 2.05718 factor:1 | 1 (-0.44278) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12071 HOMO: -6.62597 LUMO: 1.70343 factor:1 | 1 (-0.33780) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20355 HOMO: -6.69400 LUMO: 2.16875 factor:1 | -1 (0.57936) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44379 HOMO: -6.63958 LUMO: 2.11977 factor:1 | 1 (-0.66088) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60115 HOMO: -6.92802 LUMO: 1.82044 factor:1 | 1 (-0.81825) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71193 HOMO: -6.56339 LUMO: 2.30480 factor:1 | 1 (-0.92902) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22368 HOMO: -6.63958 LUMO: 1.91024 factor:1 | 1 (-0.44077) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78448 HOMO: -6.93074 LUMO: 2.05446 factor:1 | 1 (-1.00157) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44453 HOMO: -6.61509 LUMO: 2.03813 factor:1 | -1 (0.33837) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.49335 HOMO: -6.61237 LUMO: 1.91296 factor:1 | -1 (0.28956) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39999 HOMO: -6.86815 LUMO: 1.95378 factor:1 | -1 (0.38292) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.42894 HOMO: -6.63686 LUMO: 1.70888 factor:1 | -1 (0.35397) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.40864 HOMO: -6.57971 LUMO: 2.20140 factor:1 | -1 (0.37427) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19370 HOMO: -6.41100 LUMO: 1.96738 factor:1 | -1 (0.58921) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12243 HOMO: -6.90081 LUMO: 1.65989 factor:1 | -1 (0.66047) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.08643 HOMO: -6.68312 LUMO: 1.97827 factor:1 | -1 (0.69648) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96786 HOMO: -6.65318 LUMO: 2.10888 factor:1 | 1 (-0.18496) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06433 HOMO: -6.62053 LUMO: 2.28848 factor:1 | 1 (-0.28142) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.54873 HOMO: -6.65863 LUMO: 2.29664 factor:1 | -1 (0.23418) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.75621 HOMO: -6.63958 LUMO: 2.07623 factor:1 | -1 (0.02669) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00822 HOMO: -6.58243 LUMO: 2.20684 factor:1 | 1 (-0.22531) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02735 HOMO: -6.59332 LUMO: 2.05174 factor:1 | 1 (-0.24444) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00718 HOMO: -6.95251 LUMO: 2.20140 factor:1 | 1 (-0.22428) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00778 HOMO: -6.84638 LUMO: 2.39732 factor:1 | 1 (-0.22487) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05935 HOMO: -6.86815 LUMO: 2.47896 factor:1 | 1 (-0.27644) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.49779 HOMO: -7.00693 LUMO: 2.43270 factor:1 | -1 (0.28512) | 1 | 1 |
| G: -6257.41721 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: 2.30208 factor:1 | -1 (0.01818) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.49057 HOMO: -6.63958 LUMO: 2.28031 factor:1 | -1 (0.29233) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43202 HOMO: -6.74570 LUMO: 2.28304 factor:1 | -1 (0.35089) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43768 HOMO: -6.78380 LUMO: 2.16331 factor:1 | -1 (0.34523) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.06463 HOMO: -6.52529 LUMO: 2.05718 factor:1 | -1 (0.71827) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.81481 HOMO: -6.41644 LUMO: 1.65445 factor:1 | -1 (0.96810) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.80771 HOMO: -6.34570 LUMO: 1.22451 factor:1 | -1 (0.97520) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96950 HOMO: -6.14433 LUMO: 1.85582 factor:1 | 1 (-0.18659) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08335 HOMO: -6.62053 LUMO: 1.92112 factor:1 | 1 (-0.30044) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17535 HOMO: -6.63414 LUMO: 1.61908 factor:1 | 1 (-0.39244) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33207 HOMO: -6.75931 LUMO: 1.87214 factor:1 | -1 (0.45084) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.49011 HOMO: -6.55794 LUMO: 1.77418 factor:1 | -1 (0.29279) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.51175 HOMO: -6.52801 LUMO: 1.82044 factor:1 | -1 (0.27116) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99322 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-0.21032) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28586 HOMO: -6.93890 LUMO: 1.81228 factor:1 | -1 (0.49704) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58554 HOMO: -6.85455 LUMO: 1.75513 factor:1 | -1 (0.19736) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01799 HOMO: -6.86815 LUMO: 1.64629 factor:1 | 1 (-0.23508) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07127 HOMO: -6.98516 LUMO: 1.84765 factor:1 | 1 (-0.28836) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14563 HOMO: -6.04637 LUMO: 1.94017 factor:1 | 1 (-0.36273) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05556 HOMO: -6.86271 LUMO: 2.11977 factor:1 | 1 (-0.27266) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30395 HOMO: -6.72938 LUMO: 2.11160 factor:1 | 1 (-0.52104) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.62168 HOMO: -7.01782 LUMO: 2.13609 factor:1 | -1 (0.16123) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96003 HOMO: -6.18515 LUMO: 2.04630 factor:1 | 1 (-0.17712) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01061 HOMO: -6.60965 LUMO: 2.17147 factor:1 | 1 (-0.22770) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08098 HOMO: -6.87360 LUMO: 2.35378 factor:1 | 1 (-0.29807) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.21965 HOMO: -6.72938 LUMO: 2.20140 factor:1 | 1 (-0.43674) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85698 HOMO: -6.88448 LUMO: 2.54154 factor:1 | 1 (-0.07407) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10721 HOMO: -6.87087 LUMO: 2.16058 factor:1 | 1 (-0.32431) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92321 HOMO: -7.11306 LUMO: 2.04085 factor:1 | 1 (-0.14030) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05524 HOMO: -6.66951 LUMO: 1.68438 factor:1 | 1 (-0.27233) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15789 HOMO: -7.08312 LUMO: 2.19324 factor:1 | -1 (0.62502) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.94518 HOMO: -6.69128 LUMO: 2.13881 factor:1 | -1 (0.83773) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04824 HOMO: -6.80285 LUMO: 2.16603 factor:1 | 1 (-0.26534) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02740 HOMO: -6.82189 LUMO: 2.46807 factor:1 | 1 (-0.24449) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04672 HOMO: -6.78652 LUMO: 2.12521 factor:1 | 1 (-0.26381) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00337 HOMO: -6.47903 LUMO: 1.70071 factor:1 | 1 (-0.22047) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03094 HOMO: -6.37019 LUMO: 1.24356 factor:1 | 1 (-0.24803) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03967 HOMO: -6.69400 LUMO: 1.67350 factor:1 | 1 (-0.25677) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.73039 HOMO: -7.51851 LUMO: 0.27756 factor:1 | -1 (0.05252) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.66603 HOMO: -6.95795 LUMO: -0.72110 factor:1 | -1 (0.11687) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77752 HOMO: -6.88720 LUMO: -0.67484 factor:1 | -1 (0.00539) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85831 HOMO: -6.83550 LUMO: -0.57144 factor:1 | 1 (-0.07540) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91202 HOMO: -6.80285 LUMO: -0.57144 factor:1 | 1 (-0.12912) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.72941 HOMO: -6.76475 LUMO: -0.53062 factor:1 | -1 (0.05350) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08182 HOMO: -6.66951 LUMO: 1.74969 factor:1 | 1 (-0.29892) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89028 HOMO: -6.53345 LUMO: 1.89935 factor:1 | 1 (-0.10738) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22928 HOMO: -6.65046 LUMO: 2.01364 factor:1 | 1 (-0.44638) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52930 HOMO: -6.64230 LUMO: 2.11977 factor:1 | -1 (0.25361) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82827 HOMO: -6.44910 LUMO: 2.13337 factor:1 | 1 (-0.04536) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12403 HOMO: -7.05591 LUMO: 1.98915 factor:1 | 1 (-0.34112) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.61003 HOMO: -7.02326 LUMO: 2.49256 factor:1 | -1 (0.17287) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58375 HOMO: -6.32937 LUMO: 2.51161 factor:1 | -1 (0.19916) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12642 HOMO: -6.96067 LUMO: 2.20140 factor:1 | 1 (-0.34352) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35562 HOMO: -6.97972 LUMO: 2.55243 factor:1 | 1 (-0.57272) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23274 HOMO: -6.72665 LUMO: 2.46535 factor:1 | 1 (-0.44983) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.21165 HOMO: -6.41917 LUMO: 2.35106 factor:1 | 1 (-0.42874) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88163 HOMO: -6.75114 LUMO: 2.32929 factor:1 | 1 (-0.09872) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00672 HOMO: -6.91713 LUMO: 2.27215 factor:1 | 1 (-0.22381) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79153 HOMO: -6.54978 LUMO: 2.00276 factor:1 | 1 (-0.00863) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84508 HOMO: -6.62325 LUMO: 2.05990 factor:1 | 1 (-0.06218) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09393 HOMO: -6.86271 LUMO: 2.14970 factor:1 | 1 (-0.31103) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19750 HOMO: -6.77564 LUMO: 2.25855 factor:1 | 1 (-0.41459) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58807 HOMO: -6.71305 LUMO: 1.94561 factor:1 | -1 (0.19483) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09336 HOMO: -6.75659 LUMO: 1.94561 factor:1 | 1 (-0.31045) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.68761 HOMO: -6.94979 LUMO: 2.33474 factor:1 | -1 (0.09529) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79880 HOMO: -6.85727 LUMO: 2.50345 factor:1 | 1 (-0.01589) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79542 HOMO: -6.87360 LUMO: 2.43270 factor:1 | 1 (-0.01252) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.73110 HOMO: -6.57427 LUMO: 2.46807 factor:1 | -1 (0.05181) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05137 HOMO: -7.16204 LUMO: 2.15242 factor:1 | 1 (-0.26847) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47876 HOMO: -6.62869 LUMO: 2.11432 factor:1 | 1 (-0.69585) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69294 HOMO: -7.05591 LUMO: 2.26671 factor:1 | 1 (-0.91003) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84535 HOMO: -7.13483 LUMO: 1.47758 factor:1 | 1 (-1.06244) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58589 HOMO: -6.72938 LUMO: 1.57282 factor:1 | 1 (-0.80298) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60540 HOMO: -6.17426 LUMO: 1.81228 factor:1 | 1 (-0.82249) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.62266 HOMO: -6.65318 LUMO: 1.93473 factor:1 | -1 (0.16025) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.63870 HOMO: -6.18515 LUMO: 2.01364 factor:1 | 1 (-0.85580) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59772 HOMO: -7.05591 LUMO: 2.13337 factor:1 | 1 (-0.81482) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55383 HOMO: -6.90897 LUMO: 2.29664 factor:1 | 1 (-0.77093) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79552 HOMO: -7.11034 LUMO: 2.17147 factor:1 | 1 (-1.01262) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.40649 HOMO: -6.82734 LUMO: 2.26671 factor:1 | -1 (0.37642) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.47501 HOMO: -6.34842 LUMO: 2.34562 factor:1 | -1 (0.30790) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98737 HOMO: -6.62053 LUMO: 2.22861 factor:1 | 1 (-0.20447) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86498 HOMO: -6.80557 LUMO: 2.07079 factor:1 | 1 (-0.08207) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94389 HOMO: -6.60692 LUMO: 2.46263 factor:1 | 1 (-0.16098) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.62715 HOMO: -7.02054 LUMO: 2.08711 factor:1 | -1 (0.15576) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85216 HOMO: -6.78652 LUMO: 2.02453 factor:1 | 1 (-0.06925) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83869 HOMO: -6.51168 LUMO: 2.06534 factor:1 | 1 (-0.05578) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93611 HOMO: -6.50080 LUMO: 2.01636 factor:1 | 1 (-0.15320) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.62160 HOMO: -6.54434 LUMO: 1.84493 factor:1 | -1 (0.16131) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04512 HOMO: -6.47087 LUMO: 1.76330 factor:1 | 1 (-0.26221) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91153 HOMO: -6.78924 LUMO: 2.39460 factor:1 | 1 (-0.12863) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96087 HOMO: -6.59876 LUMO: 1.84493 factor:1 | 1 (-0.17796) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87172 HOMO: -6.41644 LUMO: 2.05174 factor:1 | 1 (-0.08882) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92000 HOMO: -6.52257 LUMO: 2.11160 factor:1 | 1 (-0.13709) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84560 HOMO: -6.90897 LUMO: 2.34018 factor:1 | 1 (-0.06270) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.60364 HOMO: -6.97428 LUMO: 1.86126 factor:1 | -1 (0.17927) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.73325 HOMO: -7.13483 LUMO: 2.14698 factor:1 | -1 (0.04966) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52173 HOMO: -7.16748 LUMO: 2.31841 factor:1 | -1 (0.26117) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89953 HOMO: -6.87087 LUMO: 2.38916 factor:1 | 1 (-1.11662) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.63043 HOMO: -6.93074 LUMO: 2.42181 factor:1 | 1 (-0.84753) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56167 HOMO: -6.90081 LUMO: 2.00276 factor:1 | 1 (-0.77876) | 1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48286 HOMO: -6.99333 LUMO: 2.03541 factor:1 | 1 (-1.69995) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.17120 HOMO: -6.89264 LUMO: 1.57554 factor:1 | 1 (-2.38829) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.30905 HOMO: -6.48175 LUMO: 1.85854 factor:1 | 1 (-2.52614) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37243 HOMO: -6.69400 LUMO: 1.62452 factor:1 | 1 (-1.58953) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.32321 HOMO: -6.50896 LUMO: 1.88303 factor:1 | 1 (-1.54030) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52593 HOMO: -6.60420 LUMO: 2.05990 factor:1 | 1 (-1.74303) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.09813 HOMO: -7.14299 LUMO: 2.07351 factor:1 | 1 (-2.31523) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.96129 HOMO: -7.06408 LUMO: 1.81228 factor:1 | 1 (-2.17838) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.13846 HOMO: -6.67495 LUMO: 1.79595 factor:1 | 1 (-2.35555) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.45589 HOMO: -6.45182 LUMO: 2.15786 factor:1 | 1 (-1.67298) | -1 | -1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.12113 HOMO: -6.93346 LUMO: 2.45719 factor:1 | 1 (-2.33822) | 1 | 1 |
| G: -6257.41721 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.58731 HOMO: -6.50080 LUMO: 2.08167 factor:1 | 1 (-2.80441) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46388 HOMO: -6.83550 LUMO: -0.67484 factor:1 | -1 (0.31903) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45544 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-0.67253) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22528 HOMO: -6.79740 LUMO: 1.91296 factor:1 | 1 (-0.44238) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.17193 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-2.38902) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.49543 HOMO: -6.62597 LUMO: -0.44082 factor:1 | 1 (-1.71252) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.37136 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-2.58846) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79645 HOMO: -6.51168 LUMO: -0.23130 factor:1 | 1 (-1.01354) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.40002 HOMO: -7.14027 LUMO: 0.49797 factor:1 | -1 (0.38289) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.52273 HOMO: -7.55660 LUMO: 0.24762 factor:1 | 1 (-0.73982) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50248 HOMO: -6.88992 LUMO: -0.64763 factor:1 | 1 (-0.71958) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40896 HOMO: -6.72665 LUMO: -0.45987 factor:1 | 1 (-0.62605) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53791 HOMO: -6.72121 LUMO: -0.58232 factor:1 | 1 (-0.75501) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92102 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-1.13812) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50765 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-0.72475) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.31839 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-1.53548) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.31583 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-1.53293) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52610 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-1.74319) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.28930 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-1.50640) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65620 HOMO: -6.79740 LUMO: -0.55511 factor:1 | 1 (-0.87330) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99082 HOMO: -6.79740 LUMO: -0.67756 factor:1 | 1 (-1.20791) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12658 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-1.34367) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99175 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-1.20884) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44431 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-0.66140) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58355 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-0.80064) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67383 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-0.89093) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.56475 HOMO: -6.59332 LUMO: -0.27211 factor:1 | -1 (0.21815) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26932 HOMO: -6.57427 LUMO: -0.16871 factor:1 | -1 (0.51359) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83972 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-1.05681) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26192 HOMO: -6.72121 LUMO: 2.00004 factor:1 | -1 (0.52099) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.95792 HOMO: -6.61509 LUMO: 1.55921 factor:1 | 1 (-1.17501) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96358 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-1.18067) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.29568 HOMO: -6.66135 LUMO: 2.02181 factor:1 | 1 (-0.51277) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.43312 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-0.65022) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17391 HOMO: -6.66679 LUMO: 1.98371 factor:1 | 1 (-0.39100) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18406 HOMO: -6.67495 LUMO: 2.04085 factor:1 | 1 (-0.40115) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13758 HOMO: -6.89809 LUMO: 1.95106 factor:1 | 1 (-0.35467) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16479 HOMO: -6.50352 LUMO: 1.88847 factor:1 | 1 (-0.38188) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.13188 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-2.34897) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.35163 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-2.56873) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.95448 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-2.17158) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.40231 HOMO: -6.65591 LUMO: 2.20684 factor:1 | 1 (-1.61940) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90943 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-1.12652) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65658 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-0.87368) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46491 HOMO: -6.53617 LUMO: 1.75241 factor:1 | -1 (0.31799) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48987 HOMO: -6.60420 LUMO: 1.78779 factor:1 | -1 (0.29304) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50251 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-0.71961) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45789 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-0.67498) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37499 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-1.59208) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93501 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-1.15210) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.98151 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-1.19861) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03251 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-1.24960) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88943 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-1.10652) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93950 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-1.15659) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35462 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-0.57171) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36714 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-0.58423) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87041 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-1.08750) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96310 HOMO: -6.90897 LUMO: 1.91296 factor:1 | 1 (-0.18019) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79710 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-1.01420) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36649 HOMO: -6.94162 LUMO: 1.73881 factor:1 | -1 (0.41642) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29909 HOMO: -6.73482 LUMO: 1.95922 factor:1 | -1 (0.48382) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24926 HOMO: -6.70489 LUMO: 2.04358 factor:1 | -1 (0.53364) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.11386 HOMO: -7.04231 LUMO: 1.79323 factor:1 | -1 (0.66905) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65636 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-0.87346) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11158 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-1.32868) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21375 HOMO: -6.94979 LUMO: 2.16603 factor:1 | -1 (0.56915) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96359 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-0.18068) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71280 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-0.92989) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83849 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-1.05558) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92521 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-1.14231) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24126 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-0.45835) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.60239 HOMO: -6.75387 LUMO: 1.72248 factor:1 | -1 (0.18052) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29014 HOMO: -6.86271 LUMO: 1.68711 factor:1 | -1 (0.49277) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.68124 HOMO: -6.84094 LUMO: 2.02997 factor:1 | -1 (0.10166) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44622 HOMO: -6.80557 LUMO: 2.02725 factor:1 | -1 (0.33669) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48192 HOMO: -6.38651 LUMO: 1.53472 factor:1 | -1 (0.30099) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11249 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-0.32958) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90008 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-0.11717) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39686 HOMO: -6.83822 LUMO: -0.65852 factor:1 | -1 (0.38605) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99897 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-0.21606) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98465 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-0.20175) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89777 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-0.11486) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95110 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-0.16819) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98846 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-0.20555) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95695 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-0.17404) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.72609 HOMO: -6.69128 LUMO: 1.70888 factor:1 | -1 (0.05682) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83183 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-0.04893) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33337 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-0.55046) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19328 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-0.41037) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.40663 HOMO: -6.64230 LUMO: 2.16058 factor:1 | -1 (0.37628) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15860 HOMO: -6.58788 LUMO: 2.10616 factor:1 | -1 (0.62431) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21857 HOMO: -7.01782 LUMO: 2.13609 factor:1 | -1 (0.56434) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20834 HOMO: -6.31304 LUMO: 2.31841 factor:1 | -1 (0.57457) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.17754 HOMO: -6.94979 LUMO: 2.07895 factor:1 | -1 (0.60537) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.08834 HOMO: -6.88992 LUMO: 2.28031 factor:1 | -1 (0.69457) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32369 HOMO: -6.66407 LUMO: 2.07623 factor:1 | -1 (0.45922) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16401 HOMO: -6.52529 LUMO: 1.70071 factor:1 | -1 (0.61890) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89379 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-0.11089) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99709 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-0.21418) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85186 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-0.06895) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95094 HOMO: -6.31304 LUMO: 2.18507 factor:1 | 1 (-0.16803) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.83870 HOMO: -6.18243 LUMO: 2.01636 factor:1 | -1 (0.94421) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.83818 HOMO: -6.99877 LUMO: 2.14970 factor:1 | -1 (0.94472) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22006 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-0.43715) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10108 HOMO: -6.36202 LUMO: 2.17419 factor:1 | 1 (-1.31817) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.21779 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-1.43488) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.84180 HOMO: -6.87360 LUMO: 2.34290 factor:1 | -1 (0.94111) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.77397 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-0.99107) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91170 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-0.12879) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62646 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-0.84355) | 1 | 1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83118 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-0.04827) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87894 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-0.09603) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.64260 HOMO: -6.64502 LUMO: 2.15786 factor:1 | -1 (0.14030) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53651 HOMO: -6.71305 LUMO: 1.91840 factor:1 | -1 (0.24640) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48418 HOMO: -6.44094 LUMO: 1.74425 factor:1 | -1 (0.29873) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57117 HOMO: -6.51985 LUMO: 1.84221 factor:1 | -1 (0.21173) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17500 HOMO: -6.63414 LUMO: -0.24762 factor:1 | 1 (-0.39209) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24885 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-0.46594) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57353 HOMO: -7.19741 LUMO: 0.58232 factor:1 | 1 (-0.79063) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25187 HOMO: -6.77019 LUMO: -0.56872 factor:1 | 1 (-0.46896) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74263 HOMO: -7.46136 LUMO: 0.28844 factor:1 | -1 (0.04027) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.59893 HOMO: -6.60420 LUMO: -0.54151 factor:1 | -1 (0.18398) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.59275 HOMO: -6.53890 LUMO: -0.46531 factor:1 | -1 (0.19015) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90056 HOMO: -6.81645 LUMO: -0.57144 factor:1 | 1 (-1.11765) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.85259 HOMO: -7.48041 LUMO: 0.28572 factor:1 | 1 (-1.06968) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50121 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-0.71830) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.20487 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-0.42197) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09989 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-0.31699) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18321 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-0.40031) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12264 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-0.33973) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46306 HOMO: -6.53617 LUMO: -0.25579 factor:1 | -1 (0.31984) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.21772 HOMO: -6.50896 LUMO: -0.25034 factor:1 | 1 (-0.43481) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44508 HOMO: -7.17564 LUMO: -0.68573 factor:1 | -1 (0.33783) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.66658 HOMO: -6.53617 LUMO: -0.30749 factor:1 | -1 (0.11633) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34899 HOMO: -6.55522 LUMO: -0.30749 factor:1 | -1 (0.43391) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.51131 HOMO: -7.05591 LUMO: -0.71022 factor:1 | -1 (0.27160) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.50960 HOMO: -7.17564 LUMO: -0.69933 factor:1 | -1 (0.27331) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29759 HOMO: -6.78380 LUMO: -0.67756 factor:1 | -1 (0.48532) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.31865 HOMO: -6.62325 LUMO: 2.02725 factor:1 | -1 (0.46425) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58481 HOMO: -6.63414 LUMO: 1.91296 factor:1 | -1 (0.19810) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00476 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-0.22185) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14425 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-0.36134) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04049 HOMO: -6.61237 LUMO: 2.11432 factor:1 | 1 (-0.25758) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48168 HOMO: -6.62053 LUMO: 2.09256 factor:1 | -1 (0.30123) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.60941 HOMO: -6.78652 LUMO: 2.13609 factor:1 | -1 (0.17350) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.64856 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-0.86565) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65577 HOMO: -6.85183 LUMO: 2.12793 factor:1 | 1 (-0.87286) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41448 HOMO: -6.81101 LUMO: 1.83949 factor:1 | 1 (-0.63158) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97910 HOMO: -6.98788 LUMO: 2.16058 factor:1 | 1 (-0.19619) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.59928 HOMO: -6.62869 LUMO: 2.00820 factor:1 | -1 (0.18362) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75019 HOMO: -6.34025 LUMO: 2.25855 factor:1 | 1 (-0.96728) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72516 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-0.94225) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69296 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-0.91006) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53726 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-0.75435) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84064 HOMO: -6.83278 LUMO: 1.53744 factor:1 | 1 (-1.05773) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65900 HOMO: -6.41917 LUMO: 1.82316 factor:1 | 1 (-0.87610) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80399 HOMO: -6.56339 LUMO: 1.63813 factor:1 | 1 (-1.02108) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59370 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-0.81079) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96656 HOMO: -6.63141 LUMO: 1.92112 factor:1 | 1 (-0.18365) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13181 HOMO: -6.83822 LUMO: 1.88847 factor:1 | 1 (-0.34890) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28335 HOMO: -6.84638 LUMO: 1.90480 factor:1 | 1 (-0.50044) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14686 HOMO: -6.82462 LUMO: 1.70888 factor:1 | 1 (-0.36395) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45818 HOMO: -6.82734 LUMO: 2.12521 factor:1 | 1 (-0.67528) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12920 HOMO: -6.94435 LUMO: 1.87214 factor:1 | 1 (-0.34629) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93759 HOMO: -6.98516 LUMO: 2.51433 factor:1 | 1 (-1.15469) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84323 HOMO: -6.74026 LUMO: 2.15514 factor:1 | 1 (-1.06032) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84344 HOMO: -6.93618 LUMO: 2.54426 factor:1 | 1 (-1.06054) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72733 HOMO: -6.28583 LUMO: 2.53610 factor:1 | 1 (-0.94443) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71226 HOMO: -6.56883 LUMO: 1.94834 factor:1 | 1 (-0.92935) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48923 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-0.70633) | 1 | 1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.66213 HOMO: -6.19059 LUMO: 1.99732 factor:1 | 1 (-0.87923) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39693 HOMO: -6.78108 LUMO: 2.03813 factor:1 | 1 (-0.61402) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48186 HOMO: -6.82189 LUMO: 1.77418 factor:1 | 1 (-0.69895) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65272 HOMO: -6.45454 LUMO: 1.78779 factor:1 | 1 (-0.86981) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65824 HOMO: -6.84366 LUMO: 1.77690 factor:1 | 1 (-0.87534) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58798 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-0.80508) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.77601 HOMO: -6.76475 LUMO: 2.40277 factor:1 | 1 (-0.99311) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73014 HOMO: -6.65863 LUMO: 1.86670 factor:1 | 1 (-0.94723) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33897 HOMO: -6.50080 LUMO: 1.93201 factor:1 | 1 (-0.55606) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08716 HOMO: -6.34842 LUMO: 1.70888 factor:1 | 1 (-0.30425) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28224 HOMO: -6.60692 LUMO: 2.20140 factor:1 | 1 (-0.49933) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30694 HOMO: -6.74026 LUMO: 2.14970 factor:1 | 1 (-0.52404) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.21391 HOMO: -6.63686 LUMO: 2.17419 factor:1 | 1 (-0.43100) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16177 HOMO: -6.81917 LUMO: 2.10072 factor:1 | 1 (-0.37886) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17600 HOMO: -6.92802 LUMO: 2.04358 factor:1 | 1 (-0.39310) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18885 HOMO: -6.56067 LUMO: -0.47620 factor:1 | 1 (-0.40594) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89114 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-1.10824) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.86004 HOMO: -6.78380 LUMO: -0.64763 factor:1 | 1 (-1.07714) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07295 HOMO: -6.51985 LUMO: -0.24490 factor:1 | 1 (-0.29005) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15358 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-0.37067) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.65412 HOMO: -7.10489 LUMO: -0.62586 factor:1 | -1 (0.12879) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10887 HOMO: -7.18108 LUMO: 0.48980 factor:1 | 1 (-0.32597) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75476 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-0.97185) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.28955 HOMO: -6.70761 LUMO: -0.54423 factor:1 | 1 (-1.50664) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.77078 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-1.98787) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.77043 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-1.98752) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.87111 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-2.08820) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29801 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-1.51510) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.50041 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-1.71750) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.91244 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-2.12954) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.50199 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-1.71908) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.04134 HOMO: -6.66951 LUMO: -0.40817 factor:1 | 1 (-2.25844) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30005 HOMO: -6.60420 LUMO: -0.19320 factor:1 | 1 (-1.51714) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.79747 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-2.01457) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.84050 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-2.05759) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.12725 HOMO: -7.27088 LUMO: 0.53334 factor:1 | 1 (-2.34434) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.90270 HOMO: -7.20013 LUMO: 0.59049 factor:1 | 1 (-2.11979) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23512 HOMO: -6.60148 LUMO: -0.20953 factor:1 | 1 (-1.45222) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.72558 HOMO: -6.69400 LUMO: -0.51974 factor:1 | 1 (-1.94268) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48778 HOMO: -7.40422 LUMO: -0.98777 factor:1 | 1 (-1.70487) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29659 HOMO: -6.88176 LUMO: -0.71022 factor:1 | 1 (-1.51369) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.42117 HOMO: -6.86271 LUMO: -0.59321 factor:1 | 1 (-1.63826) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30571 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-1.52280) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96056 HOMO: -6.71033 LUMO: 1.57010 factor:1 | 1 (-1.17765) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10065 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-1.31774) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11431 HOMO: -6.67495 LUMO: 2.03813 factor:1 | 1 (-1.33140) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15066 HOMO: -6.54434 LUMO: 1.83677 factor:1 | 1 (-1.36775) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20723 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-1.42433) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23654 HOMO: -6.76747 LUMO: 1.87759 factor:1 | 1 (-1.45363) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.00091 HOMO: -6.58243 LUMO: 1.61364 factor:1 | 1 (-2.21800) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.73165 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-1.94874) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.96580 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-2.18290) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25042 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-1.46751) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.34876 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-1.56585) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92528 HOMO: -6.83278 LUMO: 1.91296 factor:1 | 1 (-0.14237) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04046 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-0.25756) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79136 HOMO: -6.50080 LUMO: 1.73337 factor:1 | 1 (-1.00845) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87267 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-1.08976) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15334 HOMO: -6.63686 LUMO: 2.20140 factor:1 | 1 (-0.37043) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30003 HOMO: -6.57427 LUMO: 1.87214 factor:1 | 1 (-0.51713) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25678 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-1.47388) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.21970 HOMO: -6.63958 LUMO: 2.04902 factor:1 | 1 (-1.43679) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29034 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-1.50743) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92988 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-0.14697) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06490 HOMO: -6.72938 LUMO: 2.28304 factor:1 | 1 (-0.28199) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86846 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-0.08555) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83781 HOMO: -6.95523 LUMO: 2.33474 factor:1 | 1 (-1.05490) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76807 HOMO: -6.59876 LUMO: 2.30480 factor:1 | 1 (-0.98516) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90227 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-1.11937) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02304 HOMO: -7.06408 LUMO: 1.99187 factor:1 | 1 (-1.24013) | 1 | 1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79120 HOMO: -6.95795 LUMO: 1.88847 factor:1 | 1 (-1.00829) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83381 HOMO: -6.85455 LUMO: 1.63813 factor:1 | 1 (-1.05090) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99351 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-1.21061) | 1 | 1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92878 HOMO: -6.91441 LUMO: 1.68983 factor:1 | 1 (-1.14587) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.53137 HOMO: -6.89809 LUMO: 2.23678 factor:1 | 1 (-1.74847) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.86368 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-2.08077) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.73358 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-1.95068) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06429 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-1.28138) | 1 | 1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.08701 HOMO: -6.94979 LUMO: 2.28031 factor:1 | 1 (-1.30411) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58389 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-1.80099) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88110 HOMO: -6.87360 LUMO: 2.40277 factor:1 | 1 (-1.09820) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73476 HOMO: -6.92802 LUMO: 1.89663 factor:1 | 1 (-0.95185) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80453 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-1.02162) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60711 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-0.82421) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.35204 HOMO: -6.54978 LUMO: 1.93201 factor:1 | -1 (0.43087) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.27784 HOMO: -6.19331 LUMO: 1.46941 factor:1 | -1 (0.50507) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.56007 HOMO: -6.55794 LUMO: 1.89663 factor:1 | -1 (0.22283) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30390 HOMO: -6.07630 LUMO: 1.94289 factor:1 | 1 (-0.52099) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99030 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-1.20740) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81920 HOMO: -6.63958 LUMO: -0.61770 factor:1 | 1 (-1.03629) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45037 HOMO: -6.81101 LUMO: -0.57960 factor:1 | 1 (-0.66747) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48303 HOMO: -6.74298 LUMO: -0.57960 factor:1 | 1 (-0.70012) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45427 HOMO: -6.63686 LUMO: -0.42994 factor:1 | -1 (0.32863) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45193 HOMO: -6.60965 LUMO: -0.41089 factor:1 | -1 (0.33097) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58043 HOMO: -6.60692 LUMO: -0.80274 factor:1 | -1 (0.20248) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03197 HOMO: -6.58788 LUMO: -0.78097 factor:1 | 1 (-0.24907) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14082 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-0.35791) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98449 HOMO: -6.63141 LUMO: -0.40545 factor:1 | 1 (-0.20158) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.47262 HOMO: -6.62053 LUMO: -0.83811 factor:1 | -1 (0.31029) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.50034 HOMO: -6.59604 LUMO: -0.35375 factor:1 | -1 (0.28256) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.41215 HOMO: -6.34297 LUMO: -0.39729 factor:1 | -1 (0.37076) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10246 HOMO: -6.67223 LUMO: 1.97827 factor:1 | -1 (0.68045) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.52395 HOMO: -6.40012 LUMO: 1.89935 factor:1 | 1 (-0.74105) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33709 HOMO: -6.74842 LUMO: 1.97283 factor:1 | 1 (-1.55418) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.26326 HOMO: -6.76747 LUMO: 2.17147 factor:1 | 1 (-1.48035) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.17261 HOMO: -6.72121 LUMO: 1.55649 factor:1 | -1 (0.61030) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65367 HOMO: -6.97700 LUMO: 2.04085 factor:1 | 1 (-0.87076) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65830 HOMO: -7.06680 LUMO: 2.04085 factor:1 | 1 (-0.87539) | 1 | 1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97205 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-0.18915) | 1 | 1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75718 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.97428) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07176 HOMO: -6.72665 LUMO: 2.20140 factor:1 | 1 (-0.28885) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18104 HOMO: -6.77291 LUMO: 2.34562 factor:1 | 1 (-0.39813) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16109 HOMO: -6.73754 LUMO: 2.00276 factor:1 | 1 (-0.37818) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16476 HOMO: -7.04231 LUMO: 1.92112 factor:1 | 1 (-0.38186) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26278 HOMO: -6.83822 LUMO: 1.72248 factor:1 | 1 (-0.47987) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13875 HOMO: -6.57971 LUMO: 2.16603 factor:1 | 1 (-0.35584) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04691 HOMO: -6.80013 LUMO: 1.88575 factor:1 | 1 (-0.26400) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14016 HOMO: -6.93618 LUMO: 2.18235 factor:1 | 1 (-0.35726) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12095 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-0.33805) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05502 HOMO: -7.06952 LUMO: 2.18507 factor:1 | 1 (-0.27211) | 1 | 1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26006 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-0.47715) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05350 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-0.27059) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08523 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-0.30232) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09777 HOMO: -7.17292 LUMO: 1.90752 factor:1 | 1 (-0.31486) | 1 | 1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94922 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-0.16632) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82302 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-0.04011) | 1 | 1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04746 HOMO: -6.85727 LUMO: 2.13609 factor:1 | 1 (-0.26455) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82310 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-0.04019) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14226 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-0.35935) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42232 HOMO: -6.67223 LUMO: 2.07351 factor:1 | 1 (-0.63941) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99584 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-0.21293) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99858 HOMO: -6.90897 LUMO: 2.28848 factor:1 | 1 (-0.21568) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.69120 HOMO: -7.04231 LUMO: 1.70071 factor:1 | -1 (0.09170) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04898 HOMO: -6.69944 LUMO: 1.94834 factor:1 | 1 (-0.26607) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10950 HOMO: -6.56067 LUMO: 2.20956 factor:1 | 1 (-0.32659) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25317 HOMO: -6.65046 LUMO: 2.06807 factor:1 | 1 (-0.47027) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12248 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-0.33957) | 1 | 1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68709 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-0.90418) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67615 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-0.89324) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.95093 HOMO: -6.85183 LUMO: 2.16058 factor:1 | 1 (-1.16802) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.95422 HOMO: -6.54706 LUMO: 1.92384 factor:1 | 1 (-1.17131) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80363 HOMO: -6.84366 LUMO: 2.48984 factor:1 | 1 (-1.02073) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94010 HOMO: -6.77291 LUMO: 2.46263 factor:1 | 1 (-1.15719) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53753 HOMO: -7.01782 LUMO: 2.31025 factor:1 | 1 (-0.75463) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10596 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-0.32305) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01905 HOMO: -6.64230 LUMO: 1.97283 factor:1 | 1 (-0.23614) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.64907 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-0.86617) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71925 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-0.93634) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78200 HOMO: -7.17020 LUMO: 2.06807 factor:1 | 1 (-0.99909) | 1 | 1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50937 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-0.72646) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87297 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-1.09006) | 1 | 1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.72702 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-1.94412) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13624 HOMO: -6.92802 LUMO: 1.99187 factor:1 | 1 (-1.35333) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.75655 HOMO: -6.69672 LUMO: 2.36739 factor:1 | 1 (-1.97364) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.00075 HOMO: -7.13755 LUMO: 2.00276 factor:1 | 1 (-1.21785) | 1 | 1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.17031 HOMO: -6.92530 LUMO: 2.25582 factor:1 | 1 (-1.38740) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.79415 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-2.01125) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39894 HOMO: -6.87904 LUMO: 1.60003 factor:1 | 1 (-1.61603) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.78569 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-2.00279) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48101 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-1.69810) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.75611 HOMO: -6.74298 LUMO: 1.47486 factor:1 | 1 (-1.97321) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58561 HOMO: -6.77019 LUMO: 1.90480 factor:1 | 1 (-1.80270) | -1 | -1 |
| G: -6257.41721 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84445 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-1.06154) | -1 | -1 |