乙二醇作为反应物的反应表19-7

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: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.02664 HOMO: -6.91169 LUMO: -0.53879 factor:1 | -1 (0.85757) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.61884 HOMO: -7.29809 LUMO: 2.83543 factor:1 | -1 (0.26537) | 1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.97738 HOMO: -6.86543 LUMO: -0.70205 factor:1 | 1 (-0.09317) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.94568 HOMO: -7.47769 LUMO: 0.31293 factor:1 | 1 (-0.06147) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.38009 HOMO: -6.63141 LUMO: -0.55511 factor:1 | -1 (0.50412) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.65612 HOMO: -6.68856 LUMO: -0.30205 factor:1 | -1 (0.22809) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.54224 HOMO: -7.22190 LUMO: 0.53334 factor:1 | -1 (0.34197) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.95695 HOMO: -6.66407 LUMO: -0.27756 factor:1 | -1 (0.92726) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80823 HOMO: -7.15659 LUMO: -0.70205 factor:1 | -1 (0.07597) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.24216 HOMO: -6.69400 LUMO: 1.67622 factor:1 | -1 (0.64205) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.97998 HOMO: -6.60420 LUMO: 2.16058 factor:1 | 1 (-1.09578) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17336 HOMO: -6.87087 LUMO: 1.88031 factor:1 | 1 (-0.28915) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.98513 HOMO: -6.60965 LUMO: -0.19864 factor:1 | 1 (-1.10092) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01308 HOMO: -7.29265 LUMO: 0.52246 factor:1 | 1 (-0.12887) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23692 HOMO: -6.86543 LUMO: -0.59593 factor:1 | 1 (-0.35271) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.04978 HOMO: -7.44504 LUMO: -1.01226 factor:1 | 1 (-1.16557) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.55709 HOMO: -6.92530 LUMO: -0.75103 factor:1 | 1 (-0.67288) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91942 HOMO: -7.10489 LUMO: 2.20412 factor:1 | 1 (-0.03521) | 1 | 1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.10855 HOMO: -6.58788 LUMO: 1.73881 factor:1 | -1 (0.77566) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.02729 HOMO: -6.64502 LUMO: 1.70343 factor:1 | 1 (-0.14308) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.94466 HOMO: -6.73754 LUMO: 1.60819 factor:1 | 1 (-1.06045) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.56419 HOMO: -6.80829 LUMO: 2.45991 factor:1 | 1 (-0.67999) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.97931 HOMO: -6.91713 LUMO: 2.43814 factor:1 | 1 (-0.09510) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.94088 HOMO: -6.60692 LUMO: 1.93745 factor:1 | 1 (-1.05667) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.57943 HOMO: -6.26134 LUMO: 1.46125 factor:1 | 1 (-0.69522) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.94750 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-0.06329) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.60166 HOMO: -6.97700 LUMO: -0.73471 factor:1 | 1 (-0.71746) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.09284 HOMO: -6.92258 LUMO: -0.70205 factor:1 | 1 (-0.20863) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.95866 HOMO: -6.83550 LUMO: -0.56872 factor:1 | 1 (-0.07445) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.24833 HOMO: -6.72121 LUMO: 1.89663 factor:1 | -1 (0.63588) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87479 HOMO: -6.73482 LUMO: 1.89935 factor:1 | -1 (0.00942) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.67055 HOMO: -6.61781 LUMO: 1.86670 factor:1 | -1 (1.21366) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.05802 HOMO: -7.01782 LUMO: 2.26399 factor:1 | -1 (0.82619) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.87593 HOMO: -7.23551 LUMO: 2.09800 factor:1 | -1 (2.00828) | 1 | 1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01156 HOMO: -7.13483 LUMO: 2.17963 factor:1 | 1 (-0.12735) | 1 | 1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.65708 HOMO: -6.22869 LUMO: 2.01092 factor:1 | -1 (1.22712) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.84233 HOMO: -6.80285 LUMO: 2.14970 factor:1 | -1 (0.04188) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.79991 HOMO: -7.21102 LUMO: 2.33746 factor:1 | -1 (0.08430) | 1 | 1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91145 HOMO: -6.39740 LUMO: 2.59597 factor:1 | 1 (-0.02724) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.07205 HOMO: -7.07768 LUMO: 2.48168 factor:1 | 1 (-0.18784) | 1 | 1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.12973 HOMO: -7.11306 LUMO: 0.90614 factor:1 | -1 (1.75448) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.81083 HOMO: -6.61781 LUMO: -2.46263 factor:1 | -1 (1.07338) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68695 HOMO: -6.96611 LUMO: 0.90614 factor:1 | -1 (0.19726) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.43514 HOMO: -6.86271 LUMO: -1.14832 factor:1 | -1 (0.44907) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68140 HOMO: -6.72665 LUMO: 0.96873 factor:1 | -1 (0.20281) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.29108 HOMO: -7.14571 LUMO: 1.05036 factor:1 | -1 (0.59313) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.90838 HOMO: -7.14299 LUMO: 0.98777 factor:1 | -1 (0.97583) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.66348 HOMO: -6.99333 LUMO: 1.05852 factor:1 | -1 (1.22073) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.84064 HOMO: -6.78924 LUMO: -1.49935 factor:1 | -1 (0.04357) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80921 HOMO: -7.13755 LUMO: 0.94151 factor:1 | -1 (0.07499) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.10993 HOMO: -6.72938 LUMO: -0.35375 factor:1 | 1 (-0.22572) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.86388 HOMO: -6.99061 LUMO: 0.82450 factor:1 | -1 (0.02033) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.14634 HOMO: -6.75114 LUMO: -0.68028 factor:1 | -1 (0.73786) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45576 HOMO: -6.40556 LUMO: -0.42722 factor:1 | -1 (0.42844) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.52639 HOMO: -7.18653 LUMO: 0.42178 factor:1 | -1 (1.35782) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.61840 HOMO: -6.63958 LUMO: -0.71294 factor:1 | -1 (2.26581) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87890 HOMO: -6.63958 LUMO: -0.71022 factor:1 | -1 (0.00531) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.86932 HOMO: -6.69672 LUMO: -0.72654 factor:1 | -1 (0.01488) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64967 HOMO: -6.56883 LUMO: -0.80274 factor:1 | -1 (0.23453) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59413 HOMO: -6.68584 LUMO: -0.56872 factor:1 | -1 (0.29007) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60826 HOMO: -6.59060 LUMO: -0.35647 factor:1 | -1 (0.27595) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.61672 HOMO: -6.72121 LUMO: -0.71838 factor:1 | -1 (0.26749) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.78384 HOMO: -6.57971 LUMO: -0.61498 factor:1 | 1 (-0.89964) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.33698 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-0.45277) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62967 HOMO: -7.14027 LUMO: 0.43266 factor:1 | -1 (0.25454) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20190 HOMO: -6.43277 LUMO: -0.44082 factor:1 | 1 (-0.31769) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36838 HOMO: -6.79468 LUMO: 0.07619 factor:1 | 1 (-0.48417) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.57002 HOMO: -6.81917 LUMO: -2.57148 factor:1 | 1 (-0.68581) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.86293 HOMO: -6.71849 LUMO: 1.30615 factor:1 | -1 (0.02128) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70861 HOMO: -6.85455 LUMO: -0.63675 factor:1 | -1 (0.17560) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30277 HOMO: -6.73210 LUMO: -1.03131 factor:1 | 1 (-0.41857) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50645 HOMO: -6.83550 LUMO: -0.58777 factor:1 | 1 (-0.62224) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45898 HOMO: -6.53073 LUMO: -0.74287 factor:1 | -1 (0.42523) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46330 HOMO: -7.18381 LUMO: -0.92791 factor:1 | -1 (0.42091) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.35614 HOMO: -6.49264 LUMO: -0.44627 factor:1 | 1 (-0.47193) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.72251 HOMO: -7.32803 LUMO: 0.41361 factor:1 | 1 (-0.83830) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52050 HOMO: -6.53073 LUMO: -0.52790 factor:1 | -1 (0.36371) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68597 HOMO: -6.54978 LUMO: -0.53062 factor:1 | -1 (0.19823) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11665 HOMO: -6.56611 LUMO: -0.37824 factor:1 | 1 (-0.23244) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.71686 HOMO: -6.57155 LUMO: -0.64219 factor:1 | -1 (0.16735) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70184 HOMO: -7.08040 LUMO: 0.45715 factor:1 | -1 (0.18237) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.84173 HOMO: -6.66679 LUMO: -0.75376 factor:1 | -1 (0.04248) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.77983 HOMO: -6.83550 LUMO: -0.99322 factor:1 | -1 (1.10437) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.47857 HOMO: -6.53345 LUMO: -0.29660 factor:1 | -1 (0.40564) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62608 HOMO: -6.65046 LUMO: 2.40549 factor:1 | -1 (0.25813) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.39519 HOMO: -6.98788 LUMO: 2.01092 factor:1 | -1 (0.48902) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77719 HOMO: -6.61781 LUMO: 1.92384 factor:1 | -1 (0.10702) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.75977 HOMO: -6.61237 LUMO: 2.06807 factor:1 | -1 (0.12444) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.40375 HOMO: -6.59060 LUMO: 1.95106 factor:1 | -1 (2.48045) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89444 HOMO: -6.48175 LUMO: 1.72248 factor:1 | 1 (-0.01023) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76758 HOMO: -6.84911 LUMO: 2.03541 factor:1 | -1 (0.11663) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.66015 HOMO: -6.50624 LUMO: 2.17147 factor:1 | -1 (0.22406) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45710 HOMO: -6.68312 LUMO: 2.08439 factor:1 | -1 (0.42711) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.61768 HOMO: -6.96067 LUMO: 1.98099 factor:1 | -1 (1.26653) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.86847 HOMO: -6.93618 LUMO: 1.85854 factor:1 | 1 (-0.98426) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91063 HOMO: -6.71305 LUMO: -0.61226 factor:1 | 1 (-0.02642) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.12857 HOMO: -7.06408 LUMO: 0.80001 factor:1 | 1 (-0.24436) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46262 HOMO: -6.52257 LUMO: 0.99049 factor:1 | -1 (0.42159) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77700 HOMO: -6.84638 LUMO: 1.10750 factor:1 | -1 (0.10721) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.92074 HOMO: -6.85455 LUMO: 0.84900 factor:1 | 1 (-1.03654) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.90108 HOMO: -6.60148 LUMO: -0.78369 factor:1 | 1 (-0.01687) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.85448 HOMO: -6.86543 LUMO: -0.93063 factor:1 | 1 (-0.97028) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17564 HOMO: -6.70489 LUMO: -0.72382 factor:1 | 1 (-0.29143) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50864 HOMO: -6.59060 LUMO: 0.31293 factor:1 | -1 (0.37557) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.28571 HOMO: -6.52257 LUMO: -0.48708 factor:1 | 1 (-0.40150) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80864 HOMO: -6.54706 LUMO: -0.48164 factor:1 | -1 (0.07557) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62970 HOMO: -7.32803 LUMO: 0.08436 factor:1 | -1 (0.25451) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.36270 HOMO: -6.77291 LUMO: -0.66940 factor:1 | -1 (0.52151) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.38619 HOMO: -6.68312 LUMO: -0.53062 factor:1 | -1 (0.49802) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89670 HOMO: -7.07768 LUMO: 0.45987 factor:1 | 1 (-0.01249) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.36447 HOMO: -6.50352 LUMO: -0.63675 factor:1 | -1 (0.51974) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.15551 HOMO: -6.48992 LUMO: -0.60681 factor:1 | 1 (-0.27130) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.43410 HOMO: -6.65318 LUMO: -0.72382 factor:1 | -1 (0.45010) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.75460 HOMO: -6.54706 LUMO: 0.24218 factor:1 | -1 (0.12961) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.09850 HOMO: -6.63958 LUMO: 0.57416 factor:1 | 1 (-0.21429) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.34879 HOMO: -6.37563 LUMO: -0.48164 factor:1 | 1 (-0.46458) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52140 HOMO: -6.64774 LUMO: -0.71838 factor:1 | -1 (0.36281) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.36531 HOMO: -7.17020 LUMO: 0.45987 factor:1 | -1 (0.51889) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.42842 HOMO: -6.86543 LUMO: -1.05036 factor:1 | -1 (0.45579) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.52971 HOMO: -6.77019 LUMO: -1.03131 factor:1 | -1 (1.35450) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36887 HOMO: -6.80285 LUMO: 1.05852 factor:1 | 1 (-0.48466) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64121 HOMO: -6.76475 LUMO: 1.01771 factor:1 | -1 (0.24300) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20963 HOMO: -6.92530 LUMO: 1.37417 factor:1 | 1 (-0.32542) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27998 HOMO: -6.98244 LUMO: 1.25989 factor:1 | -1 (0.60423) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91847 HOMO: -6.74842 LUMO: 0.89798 factor:1 | 1 (-0.03426) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.77797 HOMO: -6.77019 LUMO: -1.17009 factor:1 | 1 (-0.89376) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.40737 HOMO: -6.78652 LUMO: 1.35785 factor:1 | 1 (-1.52316) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.15749 HOMO: -6.82734 LUMO: -0.68301 factor:1 | 1 (-0.27328) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.62558 HOMO: -6.48175 LUMO: -2.19052 factor:1 | 1 (-0.74137) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.41448 HOMO: -6.65863 LUMO: -0.77008 factor:1 | 1 (-0.53027) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.48097 HOMO: -6.44094 LUMO: -2.20956 factor:1 | 1 (-1.59676) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.84379 HOMO: -6.59876 LUMO: -0.57688 factor:1 | 1 (-0.95958) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.48689 HOMO: -6.78380 LUMO: -0.77008 factor:1 | 1 (-0.60268) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.99975 HOMO: -7.30354 LUMO: 0.25034 factor:1 | 1 (-0.11554) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46333 HOMO: -6.59332 LUMO: -0.53334 factor:1 | -1 (0.42088) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.91280 HOMO: -6.64230 LUMO: -0.55783 factor:1 | 1 (-1.02859) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11510 HOMO: -7.26544 LUMO: 0.20409 factor:1 | 1 (-0.23089) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.63297 HOMO: -6.61237 LUMO: -0.65307 factor:1 | 1 (-1.74877) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.93868 HOMO: -6.72393 LUMO: -0.65307 factor:1 | 1 (-1.05447) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.52000 HOMO: -6.29671 LUMO: -0.39729 factor:1 | 1 (-0.63579) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.72120 HOMO: -6.75387 LUMO: -0.53334 factor:1 | 1 (-0.83700) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.18657 HOMO: -6.53073 LUMO: -0.31293 factor:1 | 1 (-1.30236) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.55840 HOMO: -6.42189 LUMO: -0.59049 factor:1 | 1 (-0.67419) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.79132 HOMO: -6.41100 LUMO: -0.29933 factor:1 | 1 (-1.90711) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.84552 HOMO: -6.57427 LUMO: -0.53879 factor:1 | 1 (-1.96132) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.38163 HOMO: -7.43143 LUMO: 0.33470 factor:1 | 1 (-0.49742) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.66313 HOMO: -6.56067 LUMO: -0.50885 factor:1 | 1 (-0.77893) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.94981 HOMO: -6.65863 LUMO: -0.76464 factor:1 | 1 (-1.06560) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.21796 HOMO: -6.32665 LUMO: -0.41906 factor:1 | 1 (-0.33375) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.03471 HOMO: -6.57699 LUMO: 1.63813 factor:1 | 1 (-1.15050) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36177 HOMO: -6.53073 LUMO: 1.71704 factor:1 | 1 (-0.47756) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.97749 HOMO: -6.86271 LUMO: 2.07351 factor:1 | 1 (-0.09328) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.08554 HOMO: -6.63686 LUMO: 1.78235 factor:1 | 1 (-1.20133) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.09860 HOMO: -6.60965 LUMO: 1.94289 factor:1 | 1 (-1.21439) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.44950 HOMO: -6.55250 LUMO: 1.89119 factor:1 | 1 (-0.56529) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01771 HOMO: -6.50624 LUMO: 1.85582 factor:1 | 1 (-0.13350) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.48778 HOMO: -6.06814 LUMO: 1.94561 factor:1 | 1 (-1.60357) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.41771 HOMO: -6.58788 LUMO: 2.01908 factor:1 | 1 (-0.53351) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.12744 HOMO: -6.74026 LUMO: 0.31293 factor:1 | 1 (-1.24323) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.29902 HOMO: -6.54434 LUMO: -0.42994 factor:1 | 1 (-0.41481) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.32243 HOMO: -6.94707 LUMO: 0.42994 factor:1 | -1 (0.56178) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36653 HOMO: -6.98516 LUMO: 0.41361 factor:1 | 1 (-0.48232) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.23562 HOMO: -6.31304 LUMO: -0.54967 factor:1 | -1 (0.64858) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30226 HOMO: -6.48447 LUMO: -0.40817 factor:1 | 1 (-0.41805) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68350 HOMO: -6.49264 LUMO: 0.29116 factor:1 | -1 (0.20071) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.73081 HOMO: -6.48719 LUMO: -0.11973 factor:1 | 1 (-0.84660) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64360 HOMO: -7.16204 LUMO: 0.44082 factor:1 | -1 (0.24060) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.55361 HOMO: -6.74842 LUMO: -0.37552 factor:1 | 1 (-0.66940) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.29576 HOMO: -6.44638 LUMO: -0.45171 factor:1 | -1 (0.58845) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57313 HOMO: -7.07496 LUMO: 0.50341 factor:1 | -1 (0.31108) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20402 HOMO: -6.79468 LUMO: 0.11429 factor:1 | 1 (-0.31982) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27168 HOMO: -6.63958 LUMO: -0.67484 factor:1 | -1 (0.61253) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.41332 HOMO: -7.08584 LUMO: 0.46259 factor:1 | -1 (0.47089) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.96192 HOMO: -6.80285 LUMO: -0.73199 factor:1 | 1 (-1.07771) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61946 HOMO: -6.44366 LUMO: -0.45443 factor:1 | 1 (-0.73525) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50501 HOMO: -6.75931 LUMO: 0.25851 factor:1 | 1 (-0.62080) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.71266 HOMO: -6.64502 LUMO: 1.79323 factor:1 | 1 (-0.82845) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20000 HOMO: -6.51168 LUMO: 1.60275 factor:1 | 1 (-0.31579) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.15173 HOMO: -6.56067 LUMO: 1.63268 factor:1 | -1 (0.73248) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.38362 HOMO: -6.56883 LUMO: 1.70615 factor:1 | 1 (-0.49941) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.41356 HOMO: -6.77836 LUMO: 1.77962 factor:1 | -1 (0.47065) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17902 HOMO: -6.38923 LUMO: 1.85854 factor:1 | 1 (-0.29481) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.55212 HOMO: -6.35658 LUMO: 2.16875 factor:1 | -1 (0.33209) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64679 HOMO: -6.83006 LUMO: 2.31025 factor:1 | -1 (0.23742) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.97625 HOMO: -6.87087 LUMO: 1.79051 factor:1 | -1 (0.90796) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.78108 HOMO: -6.56339 LUMO: 2.37828 factor:1 | -1 (0.10313) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.83139 HOMO: -6.30488 LUMO: 2.51705 factor:1 | -1 (0.05282) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.18915 HOMO: -6.69400 LUMO: 1.95650 factor:1 | -1 (0.69506) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68897 HOMO: -6.51168 LUMO: 2.03541 factor:1 | -1 (0.19524) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.48445 HOMO: -6.30760 LUMO: 1.65173 factor:1 | -1 (0.39976) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.82630 HOMO: -6.55250 LUMO: 1.90752 factor:1 | -1 (0.05791) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85049 HOMO: -6.41372 LUMO: 1.76058 factor:1 | -1 (0.03371) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60619 HOMO: -6.23957 LUMO: 2.06534 factor:1 | -1 (0.27802) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.96493 HOMO: -6.58243 LUMO: 2.11705 factor:1 | -1 (0.91928) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64513 HOMO: -6.37835 LUMO: 2.09256 factor:1 | -1 (0.23908) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91517 HOMO: -6.50624 LUMO: 2.55787 factor:1 | 1 (-0.03097) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77659 HOMO: -6.45454 LUMO: 1.87214 factor:1 | -1 (0.10762) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.22588 HOMO: -6.53617 LUMO: 1.95650 factor:1 | -1 (0.65833) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76018 HOMO: -6.51985 LUMO: 1.71432 factor:1 | -1 (0.12403) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69691 HOMO: -6.75114 LUMO: 1.84493 factor:1 | -1 (0.18730) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50779 HOMO: -6.06270 LUMO: 1.65717 factor:1 | -1 (0.37642) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.78617 HOMO: -5.89671 LUMO: 1.71704 factor:1 | -1 (0.09804) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85038 HOMO: -6.18787 LUMO: 1.91840 factor:1 | -1 (0.03382) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.10897 HOMO: -6.01644 LUMO: 1.85582 factor:1 | 1 (-1.22476) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23409 HOMO: -6.05998 LUMO: 2.33474 factor:1 | 1 (-0.34988) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.62047 HOMO: -6.05725 LUMO: 2.03541 factor:1 | 1 (-0.73626) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.74325 HOMO: -6.80829 LUMO: 1.90480 factor:1 | -1 (0.14095) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.66594 HOMO: -6.76475 LUMO: 2.20956 factor:1 | 1 (-0.78173) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57038 HOMO: -6.29944 LUMO: 1.77962 factor:1 | -1 (0.31383) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.90790 HOMO: -6.47359 LUMO: -0.25579 factor:1 | 1 (-1.02369) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01553 HOMO: -6.57699 LUMO: -0.47348 factor:1 | 1 (-0.13132) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.80085 HOMO: -7.20830 LUMO: 0.49797 factor:1 | 1 (-0.91664) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80086 HOMO: -7.49402 LUMO: 0.29933 factor:1 | -1 (0.08335) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50333 HOMO: -6.66679 LUMO: -0.58777 factor:1 | -1 (0.38088) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.71781 HOMO: -6.67767 LUMO: -0.56328 factor:1 | -1 (0.16640) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.78820 HOMO: -7.42871 LUMO: 0.35647 factor:1 | 1 (-0.90399) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.29681 HOMO: -6.56067 LUMO: -0.54423 factor:1 | 1 (-0.41261) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50899 HOMO: -6.56339 LUMO: -0.50341 factor:1 | -1 (0.37522) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.03004 HOMO: -6.56067 LUMO: -0.48436 factor:1 | -1 (0.85417) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59835 HOMO: -6.73210 LUMO: 1.75241 factor:1 | -1 (0.28586) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.52210 HOMO: -6.48175 LUMO: 1.91296 factor:1 | 1 (-0.63789) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.37761 HOMO: -6.67767 LUMO: 1.70343 factor:1 | -1 (0.50659) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.96747 HOMO: -6.37835 LUMO: 1.96466 factor:1 | 1 (-1.08326) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.56051 HOMO: -6.40828 LUMO: 2.10072 factor:1 | 1 (-1.67630) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.41821 HOMO: -6.06542 LUMO: 1.92112 factor:1 | -1 (0.46599) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.71622 HOMO: -6.90353 LUMO: 1.83133 factor:1 | 1 (-0.83202) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.48064 HOMO: -6.37019 LUMO: 1.92929 factor:1 | -1 (1.40356) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.72281 HOMO: -6.61509 LUMO: 2.11160 factor:1 | 1 (-0.83860) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.93552 HOMO: -6.82734 LUMO: 1.77146 factor:1 | 1 (-1.05131) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64282 HOMO: -6.01100 LUMO: 1.89935 factor:1 | -1 (0.24139) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60178 HOMO: -6.49536 LUMO: 1.75241 factor:1 | -1 (0.28243) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62126 HOMO: -6.34297 LUMO: 1.86398 factor:1 | -1 (0.26294) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.51776 HOMO: -6.53073 LUMO: 1.84493 factor:1 | 1 (-1.63355) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61864 HOMO: -6.53345 LUMO: 2.41093 factor:1 | 1 (-0.73444) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.21066 HOMO: -7.01237 LUMO: 2.06262 factor:1 | 1 (-0.32645) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.67475 HOMO: -6.17154 LUMO: 1.89119 factor:1 | 1 (-0.79055) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.24073 HOMO: -6.08719 LUMO: 1.74425 factor:1 | 1 (-0.35652) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.85606 HOMO: -6.69672 LUMO: 1.95106 factor:1 | 1 (-0.97185) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.44547 HOMO: -6.58243 LUMO: 2.24766 factor:1 | 1 (-0.56126) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.64594 HOMO: -6.74570 LUMO: 2.02181 factor:1 | 1 (-0.76173) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.26122 HOMO: -6.53890 LUMO: 1.92929 factor:1 | 1 (-0.37701) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.43488 HOMO: -6.03276 LUMO: 1.67078 factor:1 | 1 (-0.55068) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45326 HOMO: -6.67767 LUMO: 2.03541 factor:1 | -1 (0.43095) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27641 HOMO: -5.98378 LUMO: 1.84221 factor:1 | -1 (0.60779) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70116 HOMO: -6.07086 LUMO: 2.01908 factor:1 | -1 (0.18305) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59963 HOMO: -6.29944 LUMO: 1.90208 factor:1 | -1 (0.28458) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59068 HOMO: -6.75114 LUMO: 1.85854 factor:1 | -1 (0.29353) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.92835 HOMO: -6.56611 LUMO: 2.49801 factor:1 | -1 (0.95585) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.65019 HOMO: -6.39740 LUMO: 1.92929 factor:1 | -1 (0.23402) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89858 HOMO: -6.85999 LUMO: -1.07757 factor:1 | 1 (-0.01437) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.44415 HOMO: -6.98244 LUMO: 1.07213 factor:1 | -1 (0.44006) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.33788 HOMO: -7.04231 LUMO: 0.64219 factor:1 | 1 (-0.45367) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.51021 HOMO: -6.96339 LUMO: 0.75648 factor:1 | -1 (0.37399) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.22642 HOMO: -6.83822 LUMO: -0.97417 factor:1 | 1 (-0.34221) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.72404 HOMO: -6.44910 LUMO: -2.15242 factor:1 | -1 (0.16017) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50015 HOMO: -6.84094 LUMO: -1.37690 factor:1 | -1 (0.38406) | -1 | -1 |
| G: -6695.51851 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.26107 HOMO: -6.74026 LUMO: -2.54699 factor:1 | -1 (0.62314) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.63887 HOMO: -6.96611 LUMO: 1.24900 factor:1 | 1 (-0.55372) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.02017 HOMO: -7.21102 LUMO: 0.82995 factor:1 | -1 (1.06497) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.96118 HOMO: -6.88448 LUMO: 0.81634 factor:1 | -1 (1.12397) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.84865 HOMO: -7.04231 LUMO: 1.10750 factor:1 | -1 (0.23649) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.03949 HOMO: -6.83550 LUMO: -0.98777 factor:1 | -1 (0.04566) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60491 HOMO: -6.82189 LUMO: 0.93879 factor:1 | 1 (-0.51976) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.94545 HOMO: -6.81101 LUMO: 0.70750 factor:1 | -1 (1.13969) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.22447 HOMO: -7.06680 LUMO: 0.74015 factor:1 | 1 (-0.13932) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.35449 HOMO: -6.68856 LUMO: 0.86260 factor:1 | -1 (0.73065) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.47621 HOMO: -6.83822 LUMO: -0.63403 factor:1 | -1 (0.60894) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.99465 HOMO: -6.84911 LUMO: 1.26533 factor:1 | -1 (1.09050) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.57031 HOMO: -7.01237 LUMO: 0.73743 factor:1 | -1 (0.51484) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.71790 HOMO: -7.00965 LUMO: 1.40139 factor:1 | -1 (0.36724) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.33816 HOMO: -6.73210 LUMO: -2.49256 factor:1 | 1 (-0.25301) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.89367 HOMO: -7.08040 LUMO: 0.84627 factor:1 | -1 (1.19148) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.38072 HOMO: -7.00965 LUMO: 0.82995 factor:1 | -1 (0.70442) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.69654 HOMO: -6.88448 LUMO: 0.82723 factor:1 | -1 (0.38861) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.62337 HOMO: -7.20013 LUMO: 0.88437 factor:1 | -1 (0.46178) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.14289 HOMO: -6.60420 LUMO: -0.53334 factor:1 | 1 (-0.05774) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.51496 HOMO: -6.78652 LUMO: -0.79729 factor:1 | -1 (0.57019) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.77865 HOMO: -6.48992 LUMO: -0.64491 factor:1 | -1 (1.30650) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.98790 HOMO: -6.85999 LUMO: -0.78097 factor:1 | -1 (1.09724) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.61189 HOMO: -6.65046 LUMO: -0.78097 factor:1 | -1 (0.47326) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.86825 HOMO: -7.24095 LUMO: 0.37280 factor:1 | -1 (1.21689) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.98287 HOMO: -6.81101 LUMO: -0.74831 factor:1 | -1 (1.10228) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.49322 HOMO: -6.69400 LUMO: -0.77280 factor:1 | -1 (0.59193) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.48845 HOMO: -6.08447 LUMO: -0.68573 factor:1 | -1 (0.59669) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.41879 HOMO: -6.66679 LUMO: -0.47076 factor:1 | -1 (0.66635) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.49959 HOMO: -6.97428 LUMO: -1.10750 factor:1 | -1 (1.58555) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.58626 HOMO: -6.69128 LUMO: -0.54151 factor:1 | -1 (1.49888) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.73620 HOMO: -6.53617 LUMO: -0.35375 factor:1 | -1 (1.34895) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.77799 HOMO: -6.75659 LUMO: -0.41361 factor:1 | -1 (1.30715) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.43230 HOMO: -6.69400 LUMO: -0.67484 factor:1 | -1 (1.65285) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.84327 HOMO: -6.89264 LUMO: -0.90886 factor:1 | -1 (1.24187) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.37588 HOMO: -6.56339 LUMO: -0.52518 factor:1 | -1 (0.70926) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.43419 HOMO: -6.45726 LUMO: -0.65852 factor:1 | -1 (0.65095) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.51915 HOMO: -6.80557 LUMO: -0.56600 factor:1 | -1 (0.56600) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.23035 HOMO: -7.19469 LUMO: -0.91702 factor:1 | -1 (0.85479) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.81380 HOMO: -6.41100 LUMO: 0.79185 factor:1 | -1 (1.27134) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.45841 HOMO: -6.39195 LUMO: 0.26123 factor:1 | -1 (0.62673) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.69975 HOMO: -6.78924 LUMO: 0.35919 factor:1 | -1 (0.38539) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.45477 HOMO: -6.50624 LUMO: 0.71838 factor:1 | -1 (0.63038) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.60867 HOMO: -6.68584 LUMO: -0.66124 factor:1 | -1 (0.47647) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.27404 HOMO: -6.45182 LUMO: -0.48980 factor:1 | -1 (1.81111) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.54278 HOMO: -7.18925 LUMO: -1.01498 factor:1 | -1 (1.54237) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.69641 HOMO: -7.18925 LUMO: -0.63130 factor:1 | -1 (1.38873) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.84360 HOMO: -6.66679 LUMO: -0.57960 factor:1 | -1 (1.24155) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.70558 HOMO: -6.44910 LUMO: -0.30205 factor:1 | -1 (1.37956) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.40652 HOMO: -7.23279 LUMO: 0.46804 factor:1 | -1 (0.67862) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.87470 HOMO: -6.92802 LUMO: -0.72927 factor:1 | -1 (1.21044) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.00730 HOMO: -6.83278 LUMO: -0.59321 factor:1 | -1 (1.07784) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.38837 HOMO: -7.44776 LUMO: 0.27211 factor:1 | -1 (0.69677) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.34170 HOMO: -6.80829 LUMO: -0.59865 factor:1 | -1 (0.74344) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.42769 HOMO: -6.63686 LUMO: -0.75103 factor:1 | -1 (0.65745) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.60675 HOMO: -6.73210 LUMO: -0.55511 factor:1 | -1 (1.47839) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.81437 HOMO: -6.50624 LUMO: 1.58642 factor:1 | -1 (1.27077) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.77655 HOMO: -6.79196 LUMO: 0.96328 factor:1 | -1 (1.30860) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.05734 HOMO: -6.82734 LUMO: 1.23540 factor:1 | -1 (0.02781) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.11902 HOMO: -6.90081 LUMO: 1.25444 factor:1 | 1 (-0.03388) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57136 HOMO: -7.00965 LUMO: -1.05036 factor:1 | 1 (-0.48621) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.43413 HOMO: -7.01237 LUMO: -1.48302 factor:1 | 1 (-0.34899) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70157 HOMO: -6.91713 LUMO: 0.93607 factor:1 | 1 (-0.61642) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.90530 HOMO: -7.02598 LUMO: 0.92247 factor:1 | 1 (-0.82015) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61590 HOMO: -6.98516 LUMO: 1.52384 factor:1 | 1 (-1.53075) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.32256 HOMO: -6.75387 LUMO: 1.04764 factor:1 | 1 (-1.23741) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.32286 HOMO: -7.09401 LUMO: 1.19458 factor:1 | 1 (-0.23772) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.32844 HOMO: -6.88992 LUMO: -1.56193 factor:1 | 1 (-0.24330) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14242 HOMO: -7.00149 LUMO: 0.99866 factor:1 | 1 (-1.05727) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.99322 HOMO: -7.13755 LUMO: 1.05308 factor:1 | 1 (-0.90807) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.22207 HOMO: -6.85183 LUMO: -1.42860 factor:1 | 1 (-0.13693) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.33846 HOMO: -6.63141 LUMO: -0.88981 factor:1 | 1 (-0.25331) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.19110 HOMO: -6.92258 LUMO: -0.82178 factor:1 | 1 (-1.10595) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17722 HOMO: -6.55794 LUMO: -0.80818 factor:1 | 1 (-1.09207) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.02557 HOMO: -6.95251 LUMO: -0.97145 factor:1 | 1 (-0.94043) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.26425 HOMO: -7.37701 LUMO: 0.14150 factor:1 | 1 (-0.17911) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.19676 HOMO: -6.74842 LUMO: -0.68028 factor:1 | 1 (-1.11161) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.94447 HOMO: -6.65046 LUMO: -0.52518 factor:1 | 1 (-1.85933) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.17552 HOMO: -6.91441 LUMO: -1.13199 factor:1 | 1 (-2.09038) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.06907 HOMO: -7.00965 LUMO: -1.00682 factor:1 | 1 (-1.98393) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.90021 HOMO: -6.55794 LUMO: -0.54967 factor:1 | 1 (-0.81506) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01561 HOMO: -6.71577 LUMO: -0.53879 factor:1 | 1 (-0.93047) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.39316 HOMO: -6.88992 LUMO: -0.55511 factor:1 | 1 (-2.30802) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.05207 HOMO: -6.74026 LUMO: -0.60681 factor:1 | 1 (-1.96692) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.34079 HOMO: -6.76747 LUMO: -0.50885 factor:1 | 1 (-1.25564) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.32166 HOMO: -6.87904 LUMO: -0.92519 factor:1 | 1 (-1.23651) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.29031 HOMO: -6.53073 LUMO: -0.53062 factor:1 | 1 (-1.20517) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.64528 HOMO: -6.97700 LUMO: -0.98505 factor:1 | 1 (-1.56014) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.64387 HOMO: -6.96884 LUMO: -0.79185 factor:1 | 1 (-1.55872) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.63356 HOMO: -6.60420 LUMO: -0.31021 factor:1 | 1 (-1.54841) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.56169 HOMO: -6.68584 LUMO: -0.63947 factor:1 | 1 (-1.47654) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.75075 HOMO: -6.41917 LUMO: -0.35103 factor:1 | 1 (-1.66561) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.72543 HOMO: -6.73482 LUMO: -0.70477 factor:1 | 1 (-0.64028) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.08680 HOMO: -6.71305 LUMO: -0.85716 factor:1 | 1 (-1.00165) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.07806 HOMO: -6.70761 LUMO: -0.63403 factor:1 | 1 (-0.99292) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61802 HOMO: -6.37563 LUMO: -0.38640 factor:1 | 1 (-1.53287) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.39189 HOMO: -6.27495 LUMO: -0.54967 factor:1 | 1 (-1.30675) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.46705 HOMO: -6.98516 LUMO: 0.38096 factor:1 | 1 (-1.38190) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50338 HOMO: -6.47087 LUMO: -0.40001 factor:1 | 1 (-1.41823) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.37259 HOMO: -6.59876 LUMO: 0.20681 factor:1 | -1 (0.71256) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.34846 HOMO: -6.89809 LUMO: 0.14966 factor:1 | 1 (-1.26332) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.27950 HOMO: -6.76203 LUMO: 2.11432 factor:1 | 1 (-2.19435) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.08262 HOMO: -6.58516 LUMO: 1.75786 factor:1 | 1 (-1.99748) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30188 HOMO: -6.37835 LUMO: 1.84493 factor:1 | 1 (-1.21673) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.99265 HOMO: -6.83550 LUMO: 1.74425 factor:1 | 1 (-0.90750) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85828 HOMO: -6.65318 LUMO: 1.79051 factor:1 | 1 (-0.77313) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.70827 HOMO: -6.68584 LUMO: 2.11160 factor:1 | -1 (0.37688) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.33518 HOMO: -6.36202 LUMO: 1.85037 factor:1 | 1 (-1.25004) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.51894 HOMO: -6.68312 LUMO: 2.23133 factor:1 | 1 (-1.43380) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.62153 HOMO: -6.66679 LUMO: 2.14154 factor:1 | 1 (-1.53638) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.23651 HOMO: -6.50896 LUMO: 1.92657 factor:1 | 1 (-2.15136) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.95772 HOMO: -6.63686 LUMO: 2.22317 factor:1 | 1 (-1.87258) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.34931 HOMO: -6.58788 LUMO: 2.17419 factor:1 | 1 (-1.26416) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36041 HOMO: -6.72665 LUMO: 2.12249 factor:1 | 1 (-1.27526) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46777 HOMO: -6.28311 LUMO: 1.91024 factor:1 | 1 (-0.38262) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.24041 HOMO: -6.56067 LUMO: 2.27487 factor:1 | 1 (-1.15526) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14253 HOMO: -6.83006 LUMO: 2.28031 factor:1 | 1 (-1.05738) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50823 HOMO: -6.45182 LUMO: 1.62724 factor:1 | 1 (-0.42308) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.40899 HOMO: -6.78380 LUMO: 1.83677 factor:1 | 1 (-0.32384) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.57270 HOMO: -6.23413 LUMO: 1.80956 factor:1 | 1 (-2.48756) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.97362 HOMO: -6.74298 LUMO: 2.16875 factor:1 | 1 (-1.88847) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.83024 HOMO: -6.81645 LUMO: 2.50073 factor:1 | 1 (-1.74509) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.81624 HOMO: -6.71033 LUMO: 1.96466 factor:1 | 1 (-2.73110) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.40586 HOMO: -6.83550 LUMO: 2.04358 factor:1 | 1 (-0.32071) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20250 HOMO: -6.60965 LUMO: 2.38100 factor:1 | 1 (-1.11735) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60290 HOMO: -6.73210 LUMO: 2.26127 factor:1 | 1 (-0.51775) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.39741 HOMO: -6.76203 LUMO: 2.13609 factor:1 | 1 (-1.31227) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.28195 HOMO: -6.71033 LUMO: 2.05990 factor:1 | 1 (-2.19680) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.46345 HOMO: -6.50896 LUMO: 2.32385 factor:1 | 1 (-2.37830) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.54953 HOMO: -6.53345 LUMO: 1.74425 factor:1 | 1 (-1.46438) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.28562 HOMO: -6.25862 LUMO: 1.63540 factor:1 | 1 (-2.20048) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.60164 HOMO: -5.90759 LUMO: 1.78779 factor:1 | 1 (-1.51649) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.41758 HOMO: -6.09807 LUMO: 1.99732 factor:1 | 1 (-1.33243) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.19841 HOMO: -5.92392 LUMO: 1.99732 factor:1 | 1 (-2.11326) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.83965 HOMO: -6.45182 LUMO: 1.72248 factor:1 | 1 (-1.75451) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.54482 HOMO: -6.53073 LUMO: 1.82588 factor:1 | 1 (-1.45967) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.94965 HOMO: -6.40828 LUMO: 2.05174 factor:1 | 1 (-0.86451) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.93248 HOMO: -6.60420 LUMO: -0.82450 factor:1 | 1 (-0.84734) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.04886 HOMO: -6.76747 LUMO: -0.57144 factor:1 | 1 (-0.96372) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05474 HOMO: -6.67767 LUMO: -0.59321 factor:1 | 1 (-0.96960) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.93931 HOMO: -6.65863 LUMO: -0.57416 factor:1 | 1 (-0.85417) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.19093 HOMO: -6.49808 LUMO: -0.54695 factor:1 | 1 (-2.10578) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.51129 HOMO: -6.50080 LUMO: -0.61498 factor:1 | 1 (-1.42615) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.51423 HOMO: -6.74842 LUMO: -0.51974 factor:1 | 1 (-1.42909) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69974 HOMO: -6.13345 LUMO: 0.67756 factor:1 | 1 (-0.61460) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.04418 HOMO: -6.48719 LUMO: 0.52790 factor:1 | 1 (-1.95903) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30291 HOMO: -6.35930 LUMO: 0.74015 factor:1 | 1 (-1.21776) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.92093 HOMO: -6.41644 LUMO: 0.22313 factor:1 | 1 (-1.83579) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.20886 HOMO: -6.85727 LUMO: -0.00272 factor:1 | 1 (-2.12371) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.36843 HOMO: -6.84638 LUMO: 0.24762 factor:1 | 1 (-2.28328) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.76123 HOMO: -6.66951 LUMO: 0.39184 factor:1 | 1 (-1.67609) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87215 HOMO: -6.62597 LUMO: -0.65035 factor:1 | 1 (-0.78701) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.87800 HOMO: -7.13755 LUMO: 0.45715 factor:1 | 1 (-1.79285) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.79724 HOMO: -7.12666 LUMO: 0.45171 factor:1 | 1 (-0.71209) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.73715 HOMO: -6.46270 LUMO: -0.46259 factor:1 | 1 (-1.65200) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.76556 HOMO: -6.36202 LUMO: -0.29660 factor:1 | 1 (-1.68041) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.84975 HOMO: -6.28583 LUMO: 0.40545 factor:1 | 1 (-1.76460) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69588 HOMO: -6.70761 LUMO: 0.41906 factor:1 | 1 (-0.61073) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.76787 HOMO: -6.76203 LUMO: -0.60954 factor:1 | 1 (-1.68272) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.51984 HOMO: -6.85999 LUMO: -0.75103 factor:1 | 1 (-1.43469) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.53419 HOMO: -7.19741 LUMO: -1.00954 factor:1 | 1 (-0.44904) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.00905 HOMO: -6.58243 LUMO: -0.33470 factor:1 | 1 (-0.92391) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.00541 HOMO: -7.22190 LUMO: 0.49253 factor:1 | 1 (-0.92026) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.38572 HOMO: -7.22462 LUMO: 0.51974 factor:1 | 1 (-0.30058) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.14954 HOMO: -7.08584 LUMO: -0.68301 factor:1 | -1 (0.93561) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.02753 HOMO: -6.68584 LUMO: -0.29660 factor:1 | 1 (-0.94238) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88380 HOMO: -6.33753 LUMO: -0.48436 factor:1 | 1 (-0.79865) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.32526 HOMO: -7.15932 LUMO: 0.55511 factor:1 | 1 (-0.24011) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01548 HOMO: -6.57427 LUMO: 2.01908 factor:1 | 1 (-0.93033) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.78048 HOMO: -6.75659 LUMO: 2.22045 factor:1 | 1 (-0.69533) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76238 HOMO: -6.73482 LUMO: 2.20956 factor:1 | 1 (-0.67724) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.13011 HOMO: -6.74026 LUMO: 1.76602 factor:1 | 1 (-2.04496) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.24772 HOMO: -6.95523 LUMO: 1.94834 factor:1 | 1 (-1.16258) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.04143 HOMO: -6.33209 LUMO: 1.87486 factor:1 | 1 (-1.95628) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.98486 HOMO: -6.71033 LUMO: 2.12521 factor:1 | 1 (-0.89972) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91267 HOMO: -6.50080 LUMO: 2.04902 factor:1 | 1 (-0.82753) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.68166 HOMO: -6.76475 LUMO: 1.94017 factor:1 | 1 (-2.59651) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.12992 HOMO: -6.53073 LUMO: 2.08983 factor:1 | 1 (-2.04477) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.64881 HOMO: -6.69944 LUMO: 2.20684 factor:1 | 1 (-2.56367) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.10682 HOMO: -6.34570 LUMO: 1.80684 factor:1 | 1 (-2.02167) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.58945 HOMO: -6.78380 LUMO: 1.95922 factor:1 | 1 (-1.50430) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.58980 HOMO: -6.93618 LUMO: 1.76058 factor:1 | 1 (-1.50465) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.08772 HOMO: -6.93346 LUMO: 1.79595 factor:1 | 1 (-1.00258) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.69851 HOMO: -6.29671 LUMO: 1.75241 factor:1 | 1 (-1.61336) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.86062 HOMO: -6.77019 LUMO: 1.74697 factor:1 | 1 (-0.77547) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.84051 HOMO: -6.87360 LUMO: 1.91024 factor:1 | 1 (-0.75536) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.09793 HOMO: -6.32665 LUMO: 1.87759 factor:1 | 1 (-1.01278) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.97599 HOMO: -6.99877 LUMO: 1.99187 factor:1 | 1 (-0.89085) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89485 HOMO: -6.72665 LUMO: 2.12521 factor:1 | 1 (-0.80970) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06778 HOMO: -6.67767 LUMO: 2.43814 factor:1 | 1 (-0.98263) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01877 HOMO: -6.99605 LUMO: 1.79051 factor:1 | 1 (-0.93362) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76984 HOMO: -6.25046 LUMO: 1.77146 factor:1 | 1 (-0.68469) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.92092 HOMO: -6.30488 LUMO: 1.90480 factor:1 | 1 (-0.83577) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.63718 HOMO: -6.38379 LUMO: 1.68438 factor:1 | 1 (-0.55204) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77204 HOMO: -6.78924 LUMO: 2.01364 factor:1 | 1 (-0.68690) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.35545 HOMO: -6.15249 LUMO: 1.98643 factor:1 | -1 (0.72970) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.85269 HOMO: -6.19331 LUMO: 2.14154 factor:1 | 1 (-1.76754) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.87609 HOMO: -6.05998 LUMO: 2.12521 factor:1 | 1 (-1.79094) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.77575 HOMO: -6.67223 LUMO: 1.91840 factor:1 | -1 (0.30939) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.20256 HOMO: -6.79196 LUMO: 2.18507 factor:1 | 1 (-0.11742) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.25694 HOMO: -6.93346 LUMO: 1.78235 factor:1 | 1 (-2.17180) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.35542 HOMO: -6.16882 LUMO: 1.80956 factor:1 | 1 (-2.27027) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.85875 HOMO: -6.72665 LUMO: 2.07895 factor:1 | 1 (-2.77360) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.56982 HOMO: -6.73210 LUMO: 1.97827 factor:1 | 1 (-2.48467) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.27461 HOMO: -6.84638 LUMO: 1.87214 factor:1 | 1 (-1.18946) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88415 HOMO: -6.83006 LUMO: 2.36195 factor:1 | 1 (-0.79901) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.83476 HOMO: -6.97700 LUMO: 1.91024 factor:1 | 1 (-0.74962) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.31880 HOMO: -6.20420 LUMO: 1.81772 factor:1 | 1 (-1.23366) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87308 HOMO: -7.09129 LUMO: 2.10344 factor:1 | 1 (-0.78793) | 1 | 1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81719 HOMO: -6.77564 LUMO: 2.14970 factor:1 | 1 (-0.73204) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.95030 HOMO: -6.81645 LUMO: 1.85854 factor:1 | 1 (-0.86516) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61810 HOMO: -6.50896 LUMO: 2.04358 factor:1 | 1 (-1.53295) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.74714 HOMO: -6.89264 LUMO: 1.66262 factor:1 | 1 (-0.66200) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.44647 HOMO: -6.75931 LUMO: 2.23950 factor:1 | 1 (-2.36132) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.30192 HOMO: -6.50080 LUMO: 1.67622 factor:1 | 1 (-2.21678) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.81203 HOMO: -6.30216 LUMO: 2.24222 factor:1 | 1 (-1.72689) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96301 HOMO: -7.18108 LUMO: 2.10072 factor:1 | 1 (-0.87787) | 1 | 1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.86390 HOMO: -6.54162 LUMO: 2.35378 factor:1 | 1 (-1.77875) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.20078 HOMO: -5.98650 LUMO: 1.48302 factor:1 | 1 (-2.11563) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.52580 HOMO: -7.15115 LUMO: 2.14970 factor:1 | 1 (-1.44065) | 1 | 1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.54095 HOMO: -6.45454 LUMO: 2.15786 factor:1 | 1 (-1.45581) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.91030 HOMO: -7.06952 LUMO: 2.14970 factor:1 | 1 (-1.82515) | 1 | 1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.91674 HOMO: -6.93618 LUMO: 1.86942 factor:1 | 1 (-1.83160) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.98486 HOMO: -6.63141 LUMO: 1.92657 factor:1 | 1 (-0.89972) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.29735 HOMO: -6.51441 LUMO: -0.44355 factor:1 | 1 (-2.21220) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.57720 HOMO: -6.82734 LUMO: -1.03131 factor:1 | 1 (-1.49205) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.52457 HOMO: -6.58788 LUMO: -0.82995 factor:1 | 1 (-1.43943) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.86817 HOMO: -6.43277 LUMO: -0.40817 factor:1 | 1 (-1.78303) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.42028 HOMO: -6.78924 LUMO: -0.72110 factor:1 | 1 (-0.33514) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.51561 HOMO: -7.28177 LUMO: 0.36735 factor:1 | -1 (0.56953) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.07045 HOMO: -6.47903 LUMO: -0.46259 factor:1 | -1 (0.01469) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.13884 HOMO: -6.67495 LUMO: -0.75376 factor:1 | 1 (-2.05370) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.15300 HOMO: -6.71033 LUMO: -0.71838 factor:1 | 1 (-1.06786) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.02703 HOMO: -6.79740 LUMO: -0.79185 factor:1 | 1 (-1.94189) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.13491 HOMO: -6.08719 LUMO: -0.63675 factor:1 | 1 (-1.04976) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.48446 HOMO: -6.84094 LUMO: 0.42994 factor:1 | 1 (-1.39932) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.61857 HOMO: -6.59604 LUMO: 0.25851 factor:1 | 1 (-0.53342) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.75225 HOMO: -6.82462 LUMO: 0.08708 factor:1 | 1 (-1.66711) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.53881 HOMO: -6.54706 LUMO: 0.44082 factor:1 | 1 (-1.45366) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.66946 HOMO: -6.99333 LUMO: 0.32109 factor:1 | 1 (-0.58431) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.39054 HOMO: -6.29944 LUMO: -0.57144 factor:1 | 1 (-0.30539) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.98159 HOMO: -6.57699 LUMO: -0.46531 factor:1 | 1 (-1.89644) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87452 HOMO: -6.24773 LUMO: -0.53879 factor:1 | 1 (-0.78938) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36873 HOMO: -6.96067 LUMO: -0.67212 factor:1 | 1 (-1.28359) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80481 HOMO: -7.24095 LUMO: -0.09252 factor:1 | 1 (-0.71966) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60643 HOMO: -6.33481 LUMO: -0.46531 factor:1 | 1 (-0.52129) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.65695 HOMO: -6.43549 LUMO: -0.33198 factor:1 | -1 (0.42820) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79799 HOMO: -6.53073 LUMO: 0.44899 factor:1 | 1 (-1.71285) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.08130 HOMO: -6.69128 LUMO: 0.47620 factor:1 | 1 (-0.99615) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.63021 HOMO: -6.65318 LUMO: 0.52246 factor:1 | 1 (-1.54506) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.38437 HOMO: -6.71305 LUMO: 0.41089 factor:1 | -1 (0.70077) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.10922 HOMO: -6.70216 LUMO: 0.19864 factor:1 | 1 (-1.02407) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14674 HOMO: -6.41100 LUMO: 0.34558 factor:1 | 1 (-1.06160) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.17071 HOMO: -7.01237 LUMO: 0.02993 factor:1 | -1 (0.91444) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.93507 HOMO: -6.85999 LUMO: 0.18776 factor:1 | 1 (-0.84992) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23368 HOMO: -6.62869 LUMO: 0.48708 factor:1 | 1 (-1.14854) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17439 HOMO: -6.43821 LUMO: -0.45715 factor:1 | 1 (-1.08924) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.16519 HOMO: -6.43277 LUMO: -0.72110 factor:1 | 1 (-1.08005) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.67919 HOMO: -7.10761 LUMO: 0.43266 factor:1 | -1 (1.40596) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57460 HOMO: -6.57699 LUMO: -0.61498 factor:1 | 1 (-0.48945) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.61140 HOMO: -6.82189 LUMO: -0.75648 factor:1 | -1 (0.47375) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.90023 HOMO: -6.55794 LUMO: -0.67212 factor:1 | -1 (1.18492) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88843 HOMO: -6.69128 LUMO: 1.88575 factor:1 | 1 (-0.80328) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.19913 HOMO: -6.65591 LUMO: 1.70888 factor:1 | 1 (-1.11398) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.75618 HOMO: -6.58788 LUMO: 1.68438 factor:1 | 1 (-0.67103) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.92394 HOMO: -6.46270 LUMO: 1.72520 factor:1 | 1 (-0.83879) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.42717 HOMO: -6.57427 LUMO: 1.73881 factor:1 | 1 (-0.34202) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.50350 HOMO: -6.45182 LUMO: 1.75241 factor:1 | -1 (0.58164) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.55722 HOMO: -6.51441 LUMO: 1.78779 factor:1 | -1 (0.52793) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.22442 HOMO: -6.67495 LUMO: 2.11705 factor:1 | -1 (0.86072) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.31417 HOMO: -6.22597 LUMO: 1.96466 factor:1 | -1 (0.77098) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52616 HOMO: -6.68040 LUMO: 2.30753 factor:1 | 1 (-0.44101) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.67061 HOMO: -6.65046 LUMO: 2.18235 factor:1 | -1 (0.41454) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.37283 HOMO: -6.38651 LUMO: 1.76874 factor:1 | -1 (0.71231) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.92392 HOMO: -6.41644 LUMO: 2.09256 factor:1 | -1 (0.16123) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.71513 HOMO: -6.14977 LUMO: 2.28031 factor:1 | 1 (-1.62999) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05575 HOMO: -6.70489 LUMO: 2.43814 factor:1 | 1 (-0.97060) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.81818 HOMO: -6.78924 LUMO: 2.27215 factor:1 | 1 (-1.73304) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.29227 HOMO: -6.86271 LUMO: 2.31025 factor:1 | 1 (-1.20712) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.08797 HOMO: -6.51168 LUMO: 2.04630 factor:1 | 1 (-1.00282) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.19039 HOMO: -6.72665 LUMO: 2.13337 factor:1 | 1 (-1.10524) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.74292 HOMO: -6.45998 LUMO: 2.16058 factor:1 | 1 (-1.65777) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14408 HOMO: -6.83822 LUMO: 2.20684 factor:1 | 1 (-1.05893) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14500 HOMO: -6.68856 LUMO: 2.19324 factor:1 | 1 (-1.05986) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80105 HOMO: -6.71577 LUMO: 2.16058 factor:1 | 1 (-0.71590) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.92046 HOMO: -6.82462 LUMO: 1.90208 factor:1 | -1 (0.16468) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.03678 HOMO: -6.61509 LUMO: 2.23950 factor:1 | 1 (-0.95164) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81645 HOMO: -6.73754 LUMO: 1.84221 factor:1 | 1 (-0.73131) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11678 HOMO: -6.56611 LUMO: 1.94561 factor:1 | 1 (-1.03164) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.27583 HOMO: -6.67767 LUMO: 1.51840 factor:1 | 1 (-1.19069) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11510 HOMO: -6.35658 LUMO: 2.16603 factor:1 | 1 (-1.02995) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.07253 HOMO: -6.35114 LUMO: 2.08983 factor:1 | -1 (1.01262) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.47333 HOMO: -6.35114 LUMO: 2.10616 factor:1 | 1 (-1.38819) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.31834 HOMO: -6.71305 LUMO: 2.01636 factor:1 | 1 (-1.23319) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81762 HOMO: -6.24773 LUMO: 1.98915 factor:1 | 1 (-0.73248) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.04264 HOMO: -6.53617 LUMO: 2.42726 factor:1 | -1 (0.04250) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.27992 HOMO: -6.59332 LUMO: 1.82316 factor:1 | 1 (-1.19477) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.02307 HOMO: -6.41372 LUMO: 1.77418 factor:1 | 1 (-0.93792) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01436 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-0.92921) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.10908 HOMO: -6.11168 LUMO: 1.70888 factor:1 | 1 (-1.02394) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62080 HOMO: -6.44910 LUMO: 2.23405 factor:1 | 1 (-0.53566) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.99608 HOMO: -6.24773 LUMO: 2.12793 factor:1 | -1 (0.08906) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.32343 HOMO: -6.07358 LUMO: 1.89663 factor:1 | 1 (-1.23828) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45862 HOMO: -6.66679 LUMO: 1.96738 factor:1 | 1 (-0.37348) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23709 HOMO: -6.68312 LUMO: 1.78235 factor:1 | 1 (-1.15194) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57179 HOMO: -6.70761 LUMO: 1.97555 factor:1 | 1 (-0.48665) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62692 HOMO: -6.15794 LUMO: 2.00548 factor:1 | 1 (-0.54178) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.66762 HOMO: -6.52257 LUMO: 1.96738 factor:1 | 1 (-1.58248) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.33769 HOMO: -6.25590 LUMO: 1.86670 factor:1 | 1 (-1.25254) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.65840 HOMO: -6.30216 LUMO: 1.84765 factor:1 | 1 (-1.57325) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.84625 HOMO: -6.76747 LUMO: 2.20956 factor:1 | 1 (-0.76110) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.51625 HOMO: -6.14161 LUMO: 1.80684 factor:1 | 1 (-1.43110) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79691 HOMO: -6.81373 LUMO: 1.91024 factor:1 | 1 (-1.71176) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05637 HOMO: -6.81917 LUMO: 2.34834 factor:1 | 1 (-0.97123) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.95108 HOMO: -6.72121 LUMO: 1.90208 factor:1 | 1 (-1.86594) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.98037 HOMO: -7.51851 LUMO: 0.26939 factor:1 | 1 (-0.89523) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.92230 HOMO: -6.65318 LUMO: -0.57144 factor:1 | 1 (-1.83715) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.69157 HOMO: -6.77564 LUMO: -0.72654 factor:1 | 1 (-1.60642) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87253 HOMO: -6.80557 LUMO: -0.60954 factor:1 | 1 (-0.78739) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.53285 HOMO: -7.35524 LUMO: 0.27483 factor:1 | 1 (-1.44770) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01246 HOMO: -6.94979 LUMO: -0.83811 factor:1 | 1 (-0.92731) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.58158 HOMO: -6.13345 LUMO: -0.67212 factor:1 | 1 (-1.49644) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.74490 HOMO: -6.47359 LUMO: -0.59321 factor:1 | 1 (-1.65976) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.63998 HOMO: -6.52257 LUMO: -0.54695 factor:1 | 1 (-1.55483) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.26777 HOMO: -6.61781 LUMO: -0.69661 factor:1 | -1 (0.81738) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.63481 HOMO: -6.77564 LUMO: -0.80001 factor:1 | 1 (-1.54966) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64986 HOMO: -7.35252 LUMO: -1.00410 factor:1 | 1 (-0.56472) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06514 HOMO: -6.35386 LUMO: -0.38912 factor:1 | 1 (-0.97999) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.72399 HOMO: -6.80285 LUMO: -0.52246 factor:1 | 1 (-0.63884) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11714 HOMO: -7.23279 LUMO: 0.30477 factor:1 | 1 (-1.03199) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.13058 HOMO: -7.13483 LUMO: -0.76192 factor:1 | 1 (-1.04543) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96761 HOMO: -6.71849 LUMO: -0.48164 factor:1 | 1 (-0.88247) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06587 HOMO: -6.85455 LUMO: -0.69389 factor:1 | 1 (-0.98073) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.28364 HOMO: -6.96339 LUMO: -0.73743 factor:1 | 1 (-1.19850) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.22283 HOMO: -7.50490 LUMO: 0.28844 factor:1 | 1 (-1.13768) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30511 HOMO: -6.63958 LUMO: -0.50069 factor:1 | 1 (-1.21997) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.37377 HOMO: -6.78924 LUMO: -0.69661 factor:1 | 1 (-1.28862) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89798 HOMO: -7.44776 LUMO: 0.33742 factor:1 | 1 (-0.81283) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.44737 HOMO: -6.15249 LUMO: 0.66396 factor:1 | 1 (-1.36223) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.29942 HOMO: -6.17426 LUMO: 0.55511 factor:1 | -1 (0.78573) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89858 HOMO: -6.83550 LUMO: 0.28844 factor:1 | 1 (-0.81343) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52850 HOMO: -6.32393 LUMO: 0.47620 factor:1 | 1 (-0.44336) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.60209 HOMO: -6.32937 LUMO: 0.45987 factor:1 | -1 (0.48306) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.37032 HOMO: -7.37429 LUMO: 0.09252 factor:1 | 1 (-0.28518) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88788 HOMO: -6.54434 LUMO: -0.39729 factor:1 | 1 (-0.80274) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.38795 HOMO: -7.35524 LUMO: 0.28028 factor:1 | 1 (-1.30280) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.37668 HOMO: -6.95523 LUMO: -0.86804 factor:1 | 1 (-1.29153) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.67181 HOMO: -6.63958 LUMO: -0.65307 factor:1 | 1 (-1.58667) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85602 HOMO: -6.73482 LUMO: -0.67212 factor:1 | 1 (-0.77087) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.72486 HOMO: -6.37835 LUMO: -0.53606 factor:1 | 1 (-0.63971) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.78096 HOMO: -6.71849 LUMO: -0.61226 factor:1 | 1 (-1.69581) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.86829 HOMO: -6.68584 LUMO: -1.11022 factor:1 | 1 (-0.78314) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.64338 HOMO: -6.80285 LUMO: -0.79185 factor:1 | 1 (-1.55823) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59332 HOMO: -7.14571 LUMO: -0.94696 factor:1 | 1 (-0.50817) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.65383 HOMO: -7.16204 LUMO: -0.66124 factor:1 | 1 (-1.56868) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.12617 HOMO: -6.54978 LUMO: -0.54967 factor:1 | 1 (-1.04103) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.99953 HOMO: -6.75114 LUMO: -0.70750 factor:1 | 1 (-0.91438) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.34129 HOMO: -7.22190 LUMO: 0.39184 factor:1 | 1 (-0.25614) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.00239 HOMO: -7.43959 LUMO: 0.30477 factor:1 | 1 (-0.91724) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.44245 HOMO: -6.87360 LUMO: -0.77552 factor:1 | 1 (-1.35730) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.46150 HOMO: -6.82734 LUMO: -0.59593 factor:1 | 1 (-1.37635) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.68420 HOMO: -6.65318 LUMO: -0.46259 factor:1 | 1 (-1.59905) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.42294 HOMO: -7.05863 LUMO: -1.17009 factor:1 | 1 (-1.33779) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.43369 HOMO: -6.57427 LUMO: -0.48708 factor:1 | 1 (-1.34854) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.70158 HOMO: -6.60420 LUMO: -0.38096 factor:1 | 1 (-1.61644) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.46052 HOMO: -6.72121 LUMO: -0.66668 factor:1 | 1 (-1.37537) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64154 HOMO: -6.52257 LUMO: -0.19320 factor:1 | 1 (-0.55639) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20498 HOMO: -6.28039 LUMO: -0.27211 factor:1 | 1 (-1.11983) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.31916 HOMO: -6.71849 LUMO: -0.42722 factor:1 | 1 (-0.23402) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.65620 HOMO: -6.27495 LUMO: 0.27756 factor:1 | 1 (-0.57106) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.68316 HOMO: -6.21780 LUMO: 0.46531 factor:1 | 1 (-1.59802) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.87035 HOMO: -6.52257 LUMO: -0.64491 factor:1 | 1 (-1.78520) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81776 HOMO: -6.73754 LUMO: 1.83133 factor:1 | 1 (-0.73261) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46567 HOMO: -6.67223 LUMO: 1.88847 factor:1 | 1 (-0.38052) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.11546 HOMO: -6.82189 LUMO: 1.59187 factor:1 | 1 (-0.03031) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.47336 HOMO: -6.43277 LUMO: 1.76330 factor:1 | 1 (-1.38822) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06737 HOMO: -6.48175 LUMO: 1.77962 factor:1 | 1 (-0.98222) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.73215 HOMO: -6.50352 LUMO: 1.68438 factor:1 | 1 (-0.64701) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58045 HOMO: -6.31576 LUMO: 2.03813 factor:1 | 1 (-0.49530) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.13409 HOMO: -6.27495 LUMO: 1.99459 factor:1 | 1 (-1.04894) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.21979 HOMO: -6.23957 LUMO: 2.17147 factor:1 | 1 (-0.13464) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23001 HOMO: -6.78108 LUMO: 2.16875 factor:1 | 1 (-1.14486) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91504 HOMO: -6.34297 LUMO: 2.10344 factor:1 | 1 (-0.82989) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60785 HOMO: -6.30216 LUMO: 2.00004 factor:1 | 1 (-0.52270) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50901 HOMO: -6.72665 LUMO: 2.09528 factor:1 | 1 (-1.42386) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.43694 HOMO: -6.86543 LUMO: 1.91568 factor:1 | -1 (0.64820) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64148 HOMO: -5.83956 LUMO: 1.89391 factor:1 | 1 (-0.55634) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06745 HOMO: -6.42189 LUMO: 2.03269 factor:1 | 1 (-0.98230) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.52240 HOMO: -6.07630 LUMO: 1.80956 factor:1 | 1 (-1.43725) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.99615 HOMO: -6.43277 LUMO: 1.81772 factor:1 | 1 (-1.91100) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.96638 HOMO: -7.03959 LUMO: 1.78779 factor:1 | 1 (-1.88123) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.67364 HOMO: -6.72121 LUMO: 2.29664 factor:1 | 1 (-1.58849) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.03794 HOMO: -6.62869 LUMO: 2.04630 factor:1 | 1 (-1.95280) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.34053 HOMO: -6.63958 LUMO: 1.84221 factor:1 | 1 (-2.25539) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.76482 HOMO: -6.70761 LUMO: 1.67350 factor:1 | 1 (-1.67968) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.23849 HOMO: -6.00283 LUMO: 1.64357 factor:1 | 1 (-2.15335) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.63066 HOMO: -6.48719 LUMO: 1.70343 factor:1 | 1 (-2.54552) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.26897 HOMO: -6.13345 LUMO: 1.44492 factor:1 | 1 (-2.18382) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76568 HOMO: -6.11168 LUMO: 1.70071 factor:1 | 1 (-0.68053) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.55027 HOMO: -6.09535 LUMO: 1.82316 factor:1 | 1 (-0.46512) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58080 HOMO: -6.81101 LUMO: 1.63540 factor:1 | 1 (-0.49566) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.98884 HOMO: -6.80013 LUMO: 2.12249 factor:1 | -1 (0.09630) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79388 HOMO: -6.48447 LUMO: 1.94561 factor:1 | 1 (-1.70874) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89009 HOMO: -6.72393 LUMO: 2.06534 factor:1 | 1 (-0.80494) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.38101 HOMO: -6.34570 LUMO: 1.98915 factor:1 | 1 (-1.29586) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.28739 HOMO: -6.31304 LUMO: 1.87759 factor:1 | 1 (-2.20224) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.73369 HOMO: -6.77564 LUMO: 1.81228 factor:1 | 1 (-1.64855) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.37131 HOMO: -6.58516 LUMO: 2.34834 factor:1 | 1 (-2.28616) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.40278 HOMO: -6.68040 LUMO: 2.20412 factor:1 | 1 (-1.31763) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.78635 HOMO: -6.20964 LUMO: 2.17147 factor:1 | 1 (-1.70120) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.00843 HOMO: -6.54706 LUMO: 2.03813 factor:1 | 1 (-0.92328) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85730 HOMO: -6.54162 LUMO: 2.17419 factor:1 | 1 (-0.77215) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.74374 HOMO: -6.75659 LUMO: 2.22589 factor:1 | 1 (-0.65860) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.49966 HOMO: -6.59604 LUMO: 2.59325 factor:1 | 1 (-0.41451) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52156 HOMO: -6.11712 LUMO: 2.02181 factor:1 | 1 (-0.43642) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69710 HOMO: -6.63141 LUMO: 2.09256 factor:1 | 1 (-0.61196) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.56265 HOMO: -6.61781 LUMO: 1.86126 factor:1 | 1 (-0.47751) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.08860 HOMO: -6.63958 LUMO: 1.77146 factor:1 | 1 (-0.00346) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91175 HOMO: -6.60420 LUMO: 1.54561 factor:1 | 1 (-0.82660) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.04214 HOMO: -6.52529 LUMO: 2.05174 factor:1 | 1 (-0.95700) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70782 HOMO: -6.80285 LUMO: 2.13609 factor:1 | 1 (-0.62268) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52477 HOMO: -6.51168 LUMO: 2.25855 factor:1 | 1 (-0.43963) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.56113 HOMO: -6.64774 LUMO: 2.46263 factor:1 | 1 (-0.47598) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.96860 HOMO: -6.40828 LUMO: 1.99732 factor:1 | -1 (0.11655) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.39513 HOMO: -5.97562 LUMO: 1.56465 factor:1 | 1 (-1.30998) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30302 HOMO: -6.75659 LUMO: 2.23405 factor:1 | 1 (-1.21787) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.71576 HOMO: -6.68584 LUMO: 2.09528 factor:1 | 1 (-1.63062) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.99762 HOMO: -6.86543 LUMO: 1.95106 factor:1 | 1 (-1.91247) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.71475 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-2.62960) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.00222 HOMO: -6.87632 LUMO: 2.08439 factor:1 | 1 (-1.91707) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.56903 HOMO: -6.33753 LUMO: 2.16603 factor:1 | 1 (-2.48388) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14680 HOMO: -6.92258 LUMO: 1.72248 factor:1 | 1 (-1.06165) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.72518 HOMO: -6.62597 LUMO: 2.10344 factor:1 | 1 (-1.64003) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.71633 HOMO: -6.63141 LUMO: 1.94017 factor:1 | 1 (-1.63119) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50887 HOMO: -6.48447 LUMO: 1.91840 factor:1 | 1 (-1.42373) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79271 HOMO: -6.41372 LUMO: 1.61364 factor:1 | 1 (-1.70757) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.18244 HOMO: -6.37291 LUMO: 1.79051 factor:1 | 1 (-2.09729) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.10341 HOMO: -6.13073 LUMO: 1.77962 factor:1 | 1 (-2.01827) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.09871 HOMO: -6.13073 LUMO: 1.98915 factor:1 | 1 (-2.01356) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.03749 HOMO: -6.44094 LUMO: 1.58370 factor:1 | 1 (-0.95234) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06182 HOMO: -6.87087 LUMO: -0.82995 factor:1 | 1 (-0.97667) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.56015 HOMO: -6.67223 LUMO: 1.08029 factor:1 | 1 (-0.47500) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.71044 HOMO: -6.82462 LUMO: 0.91702 factor:1 | 1 (-0.62529) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06837 HOMO: -6.65863 LUMO: 1.52656 factor:1 | 1 (-0.98323) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.00930 HOMO: -6.78924 LUMO: 0.86260 factor:1 | 1 (-0.92415) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58905 HOMO: -6.68584 LUMO: 0.94424 factor:1 | 1 (-0.50390) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62431 HOMO: -6.58788 LUMO: 1.00138 factor:1 | 1 (-0.53917) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77846 HOMO: -6.79740 LUMO: 0.91430 factor:1 | 1 (-0.69332) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.12867 HOMO: -6.67223 LUMO: 0.80274 factor:1 | 1 (-2.04352) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.09098 HOMO: -6.95251 LUMO: 0.90614 factor:1 | 1 (-2.00583) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.49044 HOMO: -7.19469 LUMO: 1.34152 factor:1 | 1 (-2.40530) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.65080 HOMO: -6.59332 LUMO: -0.76464 factor:1 | 1 (-2.56565) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.52835 HOMO: -6.77564 LUMO: -0.90886 factor:1 | 1 (-2.44320) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.36824 HOMO: -6.57971 LUMO: -0.41633 factor:1 | 1 (-2.28309) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.68802 HOMO: -6.68856 LUMO: -0.58232 factor:1 | 1 (-2.60288) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.67687 HOMO: -6.87087 LUMO: -0.71022 factor:1 | 1 (-2.59172) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.73821 HOMO: -6.67767 LUMO: -0.74559 factor:1 | 1 (-1.65306) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.48190 HOMO: -6.68040 LUMO: -0.65307 factor:1 | 1 (-2.39675) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.88447 HOMO: -6.32937 LUMO: 0.80274 factor:1 | 1 (-1.79933) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.04639 HOMO: -6.29671 LUMO: 0.82723 factor:1 | 1 (-0.96124) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05444 HOMO: -6.67767 LUMO: 0.59321 factor:1 | 1 (-0.96930) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58086 HOMO: -6.77836 LUMO: 0.50341 factor:1 | 1 (-0.49571) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68521 HOMO: -6.61781 LUMO: 0.42450 factor:1 | 1 (-0.60007) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.53095 HOMO: -6.83278 LUMO: 0.39457 factor:1 | 1 (-0.44580) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.34662 HOMO: -6.56883 LUMO: 0.64219 factor:1 | 1 (-0.26147) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17540 HOMO: -6.71577 LUMO: 0.40001 factor:1 | 1 (-1.09025) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.17830 HOMO: -6.86543 LUMO: -0.74287 factor:1 | 1 (-2.09315) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.32792 HOMO: -6.68584 LUMO: -0.69389 factor:1 | 1 (-1.24277) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.05574 HOMO: -6.61237 LUMO: -0.48980 factor:1 | 1 (-1.97059) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.31724 HOMO: -6.80285 LUMO: -0.58232 factor:1 | 1 (-2.23210) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.46084 HOMO: -6.88992 LUMO: -0.70205 factor:1 | 1 (-1.37570) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.31924 HOMO: -6.95251 LUMO: -0.71838 factor:1 | 1 (-1.23409) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.01220 HOMO: -7.52123 LUMO: 0.27211 factor:1 | 1 (-1.92706) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50452 HOMO: -6.76747 LUMO: -0.74015 factor:1 | 1 (-1.41937) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.66818 HOMO: -6.55250 LUMO: -0.49797 factor:1 | 1 (-0.58303) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.72578 HOMO: -6.50896 LUMO: -0.46804 factor:1 | 1 (-0.64064) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.63538 HOMO: -7.45320 LUMO: 0.08436 factor:1 | 1 (-1.55023) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.04173 HOMO: -6.82462 LUMO: -0.70477 factor:1 | 1 (-1.95658) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79759 HOMO: -6.57155 LUMO: -0.43538 factor:1 | 1 (-1.71244) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76706 HOMO: -6.72665 LUMO: -0.55239 factor:1 | 1 (-0.68192) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59792 HOMO: -7.05319 LUMO: -1.08573 factor:1 | 1 (-0.51277) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.70390 HOMO: -6.56067 LUMO: -0.45715 factor:1 | 1 (-1.61875) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.78368 HOMO: -6.76475 LUMO: -0.53879 factor:1 | 1 (-1.69853) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.42952 HOMO: -6.67223 LUMO: -0.45987 factor:1 | 1 (-1.34438) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.76266 HOMO: -6.44094 LUMO: -0.72110 factor:1 | -1 (0.32248) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.66984 HOMO: -6.66951 LUMO: -0.67756 factor:1 | 1 (-0.58469) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.37815 HOMO: -6.69400 LUMO: -0.62858 factor:1 | 1 (-1.29300) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.51881 HOMO: -6.51985 LUMO: -0.37007 factor:1 | 1 (-0.43367) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.91049 HOMO: -5.98378 LUMO: 0.78641 factor:1 | 1 (-1.82534) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.07384 HOMO: -6.11440 LUMO: 0.71294 factor:1 | 1 (-1.98869) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45810 HOMO: -6.45182 LUMO: 0.63947 factor:1 | 1 (-0.37296) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61617 HOMO: -6.78924 LUMO: 0.37007 factor:1 | 1 (-1.53102) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.04017 HOMO: -6.63686 LUMO: 0.54423 factor:1 | -1 (0.04498) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.30123 HOMO: -6.66679 LUMO: 0.48708 factor:1 | 1 (-0.21609) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.87318 HOMO: -6.81917 LUMO: 0.31021 factor:1 | 1 (-1.78803) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.45252 HOMO: -6.28583 LUMO: 0.44899 factor:1 | 1 (-1.36737) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.04880 HOMO: -6.61237 LUMO: 0.49525 factor:1 | 1 (-1.96366) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.59189 HOMO: -7.08857 LUMO: 0.38368 factor:1 | 1 (-1.50675) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.77973 HOMO: -6.53890 LUMO: -0.68845 factor:1 | 1 (-1.69459) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17442 HOMO: -6.56611 LUMO: -0.66396 factor:1 | 1 (-1.08927) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57982 HOMO: -6.04909 LUMO: -0.59865 factor:1 | 1 (-0.49468) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68630 HOMO: -6.74842 LUMO: -0.77825 factor:1 | 1 (-0.60115) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.45831 HOMO: -6.82462 LUMO: -0.61498 factor:1 | 1 (-1.37317) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.28711 HOMO: -7.40694 LUMO: 0.32926 factor:1 | 1 (-0.20196) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58747 HOMO: -6.80557 LUMO: -0.57416 factor:1 | 1 (-0.50232) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.86653 HOMO: -6.76747 LUMO: -0.67484 factor:1 | -1 (0.21862) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88976 HOMO: -7.23279 LUMO: 0.48980 factor:1 | 1 (-0.80461) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.37310 HOMO: -6.62869 LUMO: -0.24762 factor:1 | 1 (-0.28795) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96312 HOMO: -6.65863 LUMO: -0.28028 factor:1 | 1 (-0.87798) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.02123 HOMO: -6.50352 LUMO: -0.44899 factor:1 | -1 (0.06392) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.71464 HOMO: -6.62053 LUMO: -0.88437 factor:1 | -1 (0.37051) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69629 HOMO: -6.73754 LUMO: -0.77825 factor:1 | 1 (-0.61114) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.92206 HOMO: -7.24639 LUMO: 0.35647 factor:1 | 1 (-0.83691) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27024 HOMO: -6.46270 LUMO: -0.48164 factor:1 | 1 (-0.18509) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.98675 HOMO: -6.14161 LUMO: -0.66396 factor:1 | -1 (0.09840) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69751 HOMO: -6.63414 LUMO: 1.51295 factor:1 | 1 (-0.61237) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05039 HOMO: -6.52529 LUMO: 1.65989 factor:1 | 1 (-0.96524) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.62327 HOMO: -6.63686 LUMO: 1.64629 factor:1 | 1 (-1.53812) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88383 HOMO: -6.49808 LUMO: 1.60003 factor:1 | 1 (-0.79868) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.55737 HOMO: -6.85183 LUMO: 1.96194 factor:1 | 1 (-0.47223) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.26983 HOMO: -6.90081 LUMO: 1.82316 factor:1 | 1 (-0.18468) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59345 HOMO: -6.20147 LUMO: 1.95106 factor:1 | 1 (-0.50831) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46572 HOMO: -7.05047 LUMO: 1.94289 factor:1 | 1 (-0.38058) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70061 HOMO: -6.11440 LUMO: 1.83949 factor:1 | 1 (-0.61547) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81909 HOMO: -6.65046 LUMO: 1.59187 factor:1 | 1 (-0.73395) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.02703 HOMO: -6.81917 LUMO: 2.41365 factor:1 | 1 (-1.94189) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.29177 HOMO: -6.40284 LUMO: 2.48984 factor:1 | 1 (-2.20663) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61236 HOMO: -7.04775 LUMO: 2.31025 factor:1 | 1 (-1.52721) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36473 HOMO: -6.64774 LUMO: 2.20140 factor:1 | 1 (-1.27959) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77212 HOMO: -6.72393 LUMO: 2.28304 factor:1 | 1 (-0.68698) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.24160 HOMO: -6.35114 LUMO: 1.84765 factor:1 | 1 (-1.15646) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.66635 HOMO: -6.41100 LUMO: 1.74697 factor:1 | 1 (-0.58121) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27451 HOMO: -6.34297 LUMO: 1.55921 factor:1 | 1 (-0.18936) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05463 HOMO: -6.31848 LUMO: 1.67622 factor:1 | 1 (-0.96949) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58706 HOMO: -6.50896 LUMO: 2.02725 factor:1 | 1 (-0.50191) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81041 HOMO: -6.28583 LUMO: 2.00548 factor:1 | 1 (-0.72527) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.75579 HOMO: -6.67495 LUMO: 1.92384 factor:1 | 1 (-1.67064) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.23822 HOMO: -6.17154 LUMO: 2.39732 factor:1 | 1 (-2.15307) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.67630 HOMO: -6.84911 LUMO: 2.24766 factor:1 | 1 (-1.59116) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.47872 HOMO: -6.77564 LUMO: 2.38372 factor:1 | 1 (-1.39358) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.69481 HOMO: -6.18243 LUMO: 2.40821 factor:1 | 1 (-1.60966) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27119 HOMO: -6.40828 LUMO: 2.22589 factor:1 | 1 (-0.18604) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.04114 HOMO: -6.74570 LUMO: 1.88303 factor:1 | -1 (0.04400) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.31160 HOMO: -6.29944 LUMO: 2.05174 factor:1 | 1 (-0.22645) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.42537 HOMO: -7.00693 LUMO: 2.16331 factor:1 | 1 (-0.34022) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.24509 HOMO: -6.89537 LUMO: 2.19596 factor:1 | 1 (-0.15995) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.26678 HOMO: -6.72665 LUMO: 2.03813 factor:1 | 1 (-0.18164) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.22085 HOMO: -6.69944 LUMO: 2.36467 factor:1 | 1 (-0.13570) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79440 HOMO: -6.92802 LUMO: 1.72792 factor:1 | 1 (-1.70926) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80168 HOMO: -6.12256 LUMO: 1.85310 factor:1 | 1 (-0.71653) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.37692 HOMO: -6.70489 LUMO: 2.20956 factor:1 | 1 (-2.29177) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.64773 HOMO: -6.94707 LUMO: 1.81500 factor:1 | 1 (-1.56259) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.39358 HOMO: -6.39468 LUMO: 1.79051 factor:1 | 1 (-1.30843) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.70537 HOMO: -6.69128 LUMO: 2.03813 factor:1 | 1 (-1.62022) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.38289 HOMO: -6.55250 LUMO: 2.00548 factor:1 | 1 (-0.29775) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.43651 HOMO: -6.24773 LUMO: 2.09256 factor:1 | -1 (0.64864) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.10047 HOMO: -6.85727 LUMO: 1.70071 factor:1 | 1 (-0.01532) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.40044 HOMO: -6.71305 LUMO: 1.72520 factor:1 | 1 (-1.31529) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.56842 HOMO: -6.81101 LUMO: 2.15514 factor:1 | 1 (-0.48327) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.37214 HOMO: -6.93618 LUMO: 1.75513 factor:1 | 1 (-0.28700) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.12261 HOMO: -6.63686 LUMO: 2.09800 factor:1 | 1 (-1.03746) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.18441 HOMO: -6.98244 LUMO: 1.72520 factor:1 | 1 (-0.09927) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.38574 HOMO: -6.37019 LUMO: 2.35923 factor:1 | 1 (-1.30060) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.49870 HOMO: -6.55794 LUMO: 2.12521 factor:1 | 1 (-0.41356) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.32858 HOMO: -6.45998 LUMO: 1.93201 factor:1 | 1 (-0.24343) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11670 HOMO: -6.71033 LUMO: 1.58370 factor:1 | 1 (-1.03156) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.55808 HOMO: -6.67223 LUMO: 1.52928 factor:1 | 1 (-0.47293) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.15156 HOMO: -6.72121 LUMO: 1.33608 factor:1 | 1 (-1.06641) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.25738 HOMO: -6.89264 LUMO: 2.08983 factor:1 | -1 (1.82776) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.97332 HOMO: -6.31032 LUMO: 2.24766 factor:1 | -1 (1.11183) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.61589 HOMO: -6.79740 LUMO: 2.09528 factor:1 | -1 (1.46925) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.92113 HOMO: -6.78108 LUMO: 2.15786 factor:1 | 1 (-0.83599) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45740 HOMO: -6.50896 LUMO: 2.15786 factor:1 | 1 (-0.37225) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.13640 HOMO: -6.56067 LUMO: 2.24494 factor:1 | 1 (-1.05126) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.99145 HOMO: -6.72938 LUMO: 2.24494 factor:1 | 1 (-0.90630) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.61928 HOMO: -6.40556 LUMO: 1.58642 factor:1 | 1 (-0.53413) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.36964 HOMO: -6.63141 LUMO: 1.66262 factor:1 | 1 (-0.28450) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.02307 HOMO: -6.97156 LUMO: 2.23678 factor:1 | 1 (-0.93792) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.13224 HOMO: -6.86271 LUMO: 1.91296 factor:1 | 1 (-1.04709) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.04271 HOMO: -6.50624 LUMO: 1.89119 factor:1 | 1 (-0.95757) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.10205 HOMO: -6.70761 LUMO: 1.56193 factor:1 | -1 (0.98309) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76168 HOMO: -6.60420 LUMO: 1.79595 factor:1 | 1 (-0.67653) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.64851 HOMO: -6.85727 LUMO: 2.26943 factor:1 | -1 (0.43663) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.11824 HOMO: -6.23413 LUMO: 1.91024 factor:1 | 1 (-2.03310) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23907 HOMO: -6.84366 LUMO: 2.01364 factor:1 | 1 (-1.15393) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.98208 HOMO: -6.63414 LUMO: 2.54971 factor:1 | 1 (-1.89693) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.07852 HOMO: -6.52257 LUMO: 2.42998 factor:1 | 1 (-0.99338) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.09800 HOMO: -6.61509 LUMO: 2.31297 factor:1 | 1 (-2.01285) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.22089 HOMO: -6.45998 LUMO: 2.23405 factor:1 | 1 (-1.13575) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.69873 HOMO: -6.86271 LUMO: 2.22317 factor:1 | 1 (-1.61358) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96549 HOMO: -6.84366 LUMO: 2.11432 factor:1 | 1 (-0.88034) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.20243 HOMO: -6.85999 LUMO: 2.44902 factor:1 | 1 (-0.11728) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.80620 HOMO: -6.73482 LUMO: 1.93745 factor:1 | -1 (0.27894) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58086 HOMO: -6.91441 LUMO: 2.32385 factor:1 | 1 (-0.49571) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.93403 HOMO: -6.16066 LUMO: 2.26399 factor:1 | 1 (-0.84889) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.57238 HOMO: -6.71305 LUMO: 2.38644 factor:1 | 1 (-1.48724) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.82689 HOMO: -7.08312 LUMO: 2.01636 factor:1 | 1 (-1.74175) | 1 | 1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14043 HOMO: -6.15249 LUMO: 1.90752 factor:1 | 1 (-1.05528) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80535 HOMO: -6.83006 LUMO: 2.25855 factor:1 | 1 (-0.72020) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.70413 HOMO: -6.77836 LUMO: 2.24766 factor:1 | -1 (0.38101) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.90834 HOMO: -6.66951 LUMO: 2.35923 factor:1 | 1 (-0.82320) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.22364 HOMO: -6.68312 LUMO: 2.30208 factor:1 | 1 (-1.13850) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.76828 HOMO: -6.49808 LUMO: 2.49801 factor:1 | -1 (1.31687) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.34349 HOMO: -6.62325 LUMO: 1.89935 factor:1 | 1 (-0.25834) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.94209 HOMO: -6.80829 LUMO: 1.91296 factor:1 | 1 (-0.85694) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.09998 HOMO: -6.64230 LUMO: 2.13065 factor:1 | 1 (-0.01483) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.76236 HOMO: -6.40556 LUMO: 1.83949 factor:1 | -1 (0.32278) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.63512 HOMO: -6.48175 LUMO: 1.72248 factor:1 | 1 (-0.54997) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69259 HOMO: -6.61781 LUMO: 2.11432 factor:1 | 1 (-0.60744) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58951 HOMO: -6.34570 LUMO: 2.22317 factor:1 | 1 (-0.50436) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.49040 HOMO: -7.00149 LUMO: 1.80139 factor:1 | 1 (-0.40526) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.90218 HOMO: -6.66951 LUMO: 2.13065 factor:1 | -1 (0.18297) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85215 HOMO: -6.54434 LUMO: 2.20140 factor:1 | 1 (-0.76701) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.20697 HOMO: -6.67767 LUMO: 2.02997 factor:1 | 1 (-0.12183) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.07647 HOMO: -6.49536 LUMO: 2.42998 factor:1 | -1 (0.00868) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62143 HOMO: -6.70761 LUMO: 2.71025 factor:1 | 1 (-0.53628) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.74631 HOMO: -6.62869 LUMO: 2.11160 factor:1 | -1 (0.33884) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01597 HOMO: -6.61781 LUMO: 2.24494 factor:1 | 1 (-0.93082) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.95011 HOMO: -6.66135 LUMO: 2.20956 factor:1 | 1 (-0.86497) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76018 HOMO: -6.95523 LUMO: 2.03813 factor:1 | 1 (-0.67503) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.89576 HOMO: -7.11578 LUMO: 2.41365 factor:1 | -1 (1.18938) | 1 | 1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60935 HOMO: -6.99061 LUMO: 2.13881 factor:1 | 1 (-0.52420) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96617 HOMO: -6.43277 LUMO: 2.01364 factor:1 | 1 (-0.88102) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.09541 HOMO: -6.79196 LUMO: 2.04358 factor:1 | -1 (0.98973) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.08568 HOMO: -7.08584 LUMO: 1.99732 factor:1 | 1 (-1.00054) | 1 | 1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.67724 HOMO: -6.46815 LUMO: 2.29936 factor:1 | 1 (-0.59209) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.58516 HOMO: -6.78108 LUMO: 1.93745 factor:1 | -1 (0.49998) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.33628 HOMO: -6.43277 LUMO: 1.80956 factor:1 | 1 (-0.25113) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.51972 HOMO: -6.71577 LUMO: -0.81090 factor:1 | -1 (0.56543) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.53351 HOMO: -7.14027 LUMO: -0.68028 factor:1 | 1 (-0.44836) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45198 HOMO: -7.03414 LUMO: -0.69661 factor:1 | 1 (-0.36684) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.37565 HOMO: -6.64502 LUMO: -0.47348 factor:1 | 1 (-0.29051) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.90829 HOMO: -6.60692 LUMO: 2.12793 factor:1 | 1 (-0.82314) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.67283 HOMO: -6.66407 LUMO: 1.94561 factor:1 | 1 (-0.58768) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96062 HOMO: -7.10217 LUMO: 1.92384 factor:1 | 1 (-0.87547) | 1 | 1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.75634 HOMO: -6.84094 LUMO: 1.66534 factor:1 | 1 (-0.67120) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.98609 HOMO: -6.93618 LUMO: 2.13065 factor:1 | 1 (-0.90094) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.78306 HOMO: -6.60692 LUMO: 2.20684 factor:1 | 1 (-0.69792) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.74805 HOMO: -6.85727 LUMO: 2.19324 factor:1 | -1 (0.33709) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.53781 HOMO: -6.31032 LUMO: 1.76330 factor:1 | 1 (-0.45266) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.55896 HOMO: -6.43821 LUMO: 2.10072 factor:1 | -1 (0.52619) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.21162 HOMO: -6.42189 LUMO: 2.19596 factor:1 | 1 (-0.12648) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.28574 HOMO: -6.40556 LUMO: 2.02181 factor:1 | -1 (1.79941) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.93187 HOMO: -6.41372 LUMO: 2.26671 factor:1 | -1 (1.15327) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.64926 HOMO: -6.60692 LUMO: 2.09800 factor:1 | -1 (1.43589) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77901 HOMO: -6.75931 LUMO: 1.76602 factor:1 | 1 (-0.69386) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57408 HOMO: -6.39195 LUMO: 1.84221 factor:1 | 1 (-0.48893) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.82932 HOMO: -6.74570 LUMO: 2.04085 factor:1 | 1 (-0.74418) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.92955 HOMO: -6.77019 LUMO: 2.16875 factor:1 | -1 (0.15559) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.78731 HOMO: -6.15522 LUMO: 1.81772 factor:1 | 1 (-0.70216) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69109 HOMO: -6.48175 LUMO: 2.02453 factor:1 | 1 (-0.60594) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.56336 HOMO: -6.57427 LUMO: 1.77962 factor:1 | 1 (-0.47821) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.97395 HOMO: -6.57699 LUMO: 2.42998 factor:1 | 1 (-0.88881) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89267 HOMO: -6.35386 LUMO: 2.25310 factor:1 | 1 (-0.80753) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.95294 HOMO: -6.80013 LUMO: 2.11160 factor:1 | 1 (-0.86780) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.19138 HOMO: -6.24229 LUMO: 2.05718 factor:1 | 1 (-0.10623) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.25718 HOMO: -6.42733 LUMO: 1.76874 factor:1 | -1 (0.82796) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.36872 HOMO: -6.56883 LUMO: 2.36195 factor:1 | 1 (-0.28357) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.50075 HOMO: -6.72665 LUMO: 2.28848 factor:1 | -1 (0.58439) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46605 HOMO: -6.39195 LUMO: 1.79051 factor:1 | 1 (-0.38090) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.27861 HOMO: -6.70761 LUMO: 0.15510 factor:1 | 1 (-1.19346) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.33692 HOMO: -6.44366 LUMO: -0.16871 factor:1 | 1 (-1.25178) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62004 HOMO: -6.68584 LUMO: 1.69527 factor:1 | 1 (-0.53489) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61992 HOMO: -6.26950 LUMO: 1.61636 factor:1 | 1 (-1.53478) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.92252 HOMO: -6.47631 LUMO: 1.98915 factor:1 | 1 (-0.83738) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.02664 HOMO: -6.58243 LUMO: 1.97283 factor:1 | -1 (0.05850) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.61884 HOMO: -6.51713 LUMO: 1.97283 factor:1 | 1 (-0.53370) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.97738 HOMO: -6.65046 LUMO: 1.69255 factor:1 | 1 (-0.89223) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.94568 HOMO: -6.26406 LUMO: 2.21773 factor:1 | 1 (-0.86053) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.38009 HOMO: -6.88992 LUMO: 2.28304 factor:1 | 1 (-0.29494) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.65612 HOMO: -6.67767 LUMO: 2.34834 factor:1 | 1 (-0.57098) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.54224 HOMO: -6.52801 LUMO: 2.10344 factor:1 | 1 (-0.45710) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.95695 HOMO: -6.52801 LUMO: 2.24222 factor:1 | -1 (0.12819) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80823 HOMO: -6.17154 LUMO: 1.89663 factor:1 | 1 (-0.72309) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.24216 HOMO: -6.42733 LUMO: 2.15514 factor:1 | 1 (-0.15701) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.97998 HOMO: -6.36474 LUMO: 2.01364 factor:1 | 1 (-1.89484) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17336 HOMO: -6.82189 LUMO: 1.86942 factor:1 | 1 (-1.08821) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.98513 HOMO: -6.60148 LUMO: 2.00548 factor:1 | 1 (-1.89998) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01308 HOMO: -6.67767 LUMO: 2.15786 factor:1 | 1 (-0.92794) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23692 HOMO: -6.79196 LUMO: 2.06534 factor:1 | 1 (-1.15178) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.04978 HOMO: -6.70216 LUMO: 1.83405 factor:1 | 1 (-1.96463) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.55709 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-1.47195) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91942 HOMO: -6.34842 LUMO: 1.80139 factor:1 | 1 (-0.83427) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.10855 HOMO: -6.48175 LUMO: 1.95922 factor:1 | 1 (-0.02340) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.02729 HOMO: -6.71033 LUMO: 2.02997 factor:1 | 1 (-0.94214) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.94466 HOMO: -6.89264 LUMO: 2.42726 factor:1 | 1 (-1.85952) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.56419 HOMO: -6.74570 LUMO: 2.20684 factor:1 | 1 (-1.47905) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.97931 HOMO: -6.30216 LUMO: 2.15242 factor:1 | 1 (-0.89417) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.94088 HOMO: -6.94979 LUMO: 2.43814 factor:1 | 1 (-1.85573) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.57943 HOMO: -6.97972 LUMO: 2.11432 factor:1 | 1 (-1.49429) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.94750 HOMO: -6.17154 LUMO: 1.98099 factor:1 | 1 (-0.86236) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.60166 HOMO: -6.74026 LUMO: 2.21501 factor:1 | 1 (-1.51652) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.09284 HOMO: -6.72393 LUMO: 2.19596 factor:1 | 1 (-1.00769) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.95866 HOMO: -6.11440 LUMO: 2.10072 factor:1 | 1 (-0.87351) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.24833 HOMO: -6.34297 LUMO: 1.92657 factor:1 | 1 (-0.16319) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87479 HOMO: -6.24773 LUMO: 2.00276 factor:1 | 1 (-0.78965) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.67055 HOMO: -6.75114 LUMO: 1.98643 factor:1 | -1 (0.41459) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.05802 HOMO: -6.69128 LUMO: 2.08711 factor:1 | -1 (0.02713) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.87593 HOMO: -6.65318 LUMO: 2.15514 factor:1 | -1 (1.20922) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01156 HOMO: -6.67495 LUMO: 1.72248 factor:1 | 1 (-0.92641) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.65708 HOMO: -6.58243 LUMO: 1.83405 factor:1 | -1 (0.42806) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.84233 HOMO: -6.61237 LUMO: 1.69799 factor:1 | 1 (-0.75718) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.79991 HOMO: -6.57427 LUMO: 2.29936 factor:1 | 1 (-0.71476) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91145 HOMO: -6.40012 LUMO: 2.35378 factor:1 | 1 (-0.82630) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.07205 HOMO: -6.90081 LUMO: 2.26671 factor:1 | 1 (-0.98690) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.12973 HOMO: -6.44910 LUMO: 2.25855 factor:1 | -1 (0.95542) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.81083 HOMO: -6.61509 LUMO: 2.26943 factor:1 | -1 (0.27432) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68695 HOMO: -6.78924 LUMO: 2.09256 factor:1 | 1 (-0.60181) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.43514 HOMO: -6.47087 LUMO: 1.97555 factor:1 | 1 (-0.34999) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68140 HOMO: -6.75931 LUMO: 1.98643 factor:1 | 1 (-0.59626) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.29108 HOMO: -6.17971 LUMO: 2.09800 factor:1 | 1 (-0.20594) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.90838 HOMO: -6.83006 LUMO: 1.91840 factor:1 | -1 (0.17677) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.66348 HOMO: -6.72938 LUMO: 2.17419 factor:1 | -1 (0.42167) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.84064 HOMO: -6.78924 LUMO: 2.42726 factor:1 | 1 (-0.75550) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80921 HOMO: -6.41372 LUMO: 1.93745 factor:1 | 1 (-0.72407) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.10993 HOMO: -6.85455 LUMO: 2.14970 factor:1 | 1 (-1.02478) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.86388 HOMO: -6.38651 LUMO: 2.18507 factor:1 | 1 (-0.77874) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.14634 HOMO: -6.81373 LUMO: 2.00548 factor:1 | 1 (-0.06120) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45576 HOMO: -6.64774 LUMO: 2.41365 factor:1 | 1 (-0.37062) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.52639 HOMO: -6.70489 LUMO: 2.31569 factor:1 | -1 (0.55876) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.61840 HOMO: -6.49264 LUMO: 1.78779 factor:1 | -1 (1.46675) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87890 HOMO: -6.81101 LUMO: 1.86670 factor:1 | 1 (-0.79376) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.86932 HOMO: -6.72121 LUMO: 1.48846 factor:1 | 1 (-0.78418) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64967 HOMO: -6.35930 LUMO: 1.78507 factor:1 | 1 (-0.56453) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59413 HOMO: -6.38651 LUMO: 2.04358 factor:1 | 1 (-0.50899) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60826 HOMO: -6.42189 LUMO: 1.99187 factor:1 | 1 (-0.52311) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.61672 HOMO: -6.69400 LUMO: 1.61091 factor:1 | 1 (-0.53157) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.78384 HOMO: -6.81101 LUMO: 2.17419 factor:1 | 1 (-1.69870) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.33698 HOMO: -6.90897 LUMO: 2.28576 factor:1 | 1 (-1.25183) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62967 HOMO: -6.75387 LUMO: 2.31297 factor:1 | 1 (-0.54453) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20190 HOMO: -7.05863 LUMO: 2.18780 factor:1 | 1 (-1.11676) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36838 HOMO: -6.56611 LUMO: 1.99187 factor:1 | 1 (-1.28323) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.57002 HOMO: -6.59060 LUMO: 1.86398 factor:1 | 1 (-1.48487) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.86293 HOMO: -6.59060 LUMO: 1.59459 factor:1 | 1 (-0.77778) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70861 HOMO: -6.57699 LUMO: 1.48030 factor:1 | 1 (-0.62347) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30277 HOMO: -6.99605 LUMO: 2.30208 factor:1 | 1 (-1.21763) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50645 HOMO: -6.42189 LUMO: 2.20412 factor:1 | 1 (-1.42131) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45898 HOMO: -7.15115 LUMO: 1.83405 factor:1 | 1 (-0.37383) | 1 | 1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46330 HOMO: -7.08040 LUMO: 2.21773 factor:1 | 1 (-0.37816) | 1 | 1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.35614 HOMO: -6.72121 LUMO: 1.89663 factor:1 | 1 (-1.27099) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.72251 HOMO: -6.25590 LUMO: 1.85037 factor:1 | 1 (-1.63736) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52050 HOMO: -6.70489 LUMO: 1.98915 factor:1 | 1 (-0.43535) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68597 HOMO: -6.53617 LUMO: 2.08439 factor:1 | 1 (-0.60083) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11665 HOMO: -6.69944 LUMO: 1.98915 factor:1 | 1 (-1.03150) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.71686 HOMO: -6.79468 LUMO: 1.96466 factor:1 | 1 (-0.63171) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70184 HOMO: -6.79468 LUMO: 1.99459 factor:1 | 1 (-0.61669) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.84173 HOMO: -6.58788 LUMO: 1.98371 factor:1 | 1 (-0.75659) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.77983 HOMO: -6.58788 LUMO: 2.16603 factor:1 | -1 (0.30531) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.47857 HOMO: -6.56883 LUMO: 1.64085 factor:1 | 1 (-0.39342) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62608 HOMO: -7.19197 LUMO: 2.66127 factor:1 | 1 (-0.54094) | 1 | 1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.39519 HOMO: -6.48175 LUMO: 2.40004 factor:1 | 1 (-0.31005) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77719 HOMO: -6.18515 LUMO: 2.27759 factor:1 | 1 (-0.69204) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.75977 HOMO: -6.64774 LUMO: 2.13337 factor:1 | 1 (-0.67462) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.40375 HOMO: -6.39740 LUMO: 1.95106 factor:1 | -1 (1.68139) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89444 HOMO: -6.59332 LUMO: 1.81772 factor:1 | 1 (-0.80929) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76758 HOMO: -6.68312 LUMO: 2.41909 factor:1 | 1 (-0.68243) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.66015 HOMO: -5.87494 LUMO: 2.18235 factor:1 | 1 (-0.57500) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45710 HOMO: -6.30488 LUMO: 2.04902 factor:1 | 1 (-0.37195) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.61768 HOMO: -6.65046 LUMO: 2.05446 factor:1 | -1 (0.46746) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.86847 HOMO: -6.55794 LUMO: 2.06807 factor:1 | 1 (-1.78333) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91063 HOMO: -6.68040 LUMO: 1.99187 factor:1 | 1 (-0.82548) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.12857 HOMO: -6.60965 LUMO: 2.18780 factor:1 | 1 (-1.04342) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46262 HOMO: -6.88176 LUMO: 2.10344 factor:1 | 1 (-0.37748) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77700 HOMO: -6.63414 LUMO: 1.70615 factor:1 | 1 (-0.69185) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.92074 HOMO: -7.15115 LUMO: 2.07351 factor:1 | 1 (-1.83560) | 1 | 1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.90108 HOMO: -6.85727 LUMO: 2.27759 factor:1 | 1 (-0.81593) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.85448 HOMO: -6.91713 LUMO: 2.28848 factor:1 | 1 (-1.76934) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17564 HOMO: -7.10217 LUMO: 2.14698 factor:1 | 1 (-1.09050) | 1 | 1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50864 HOMO: -6.78108 LUMO: 2.45447 factor:1 | 1 (-0.42349) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.28571 HOMO: -6.78380 LUMO: 2.43542 factor:1 | 1 (-1.20057) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80864 HOMO: -6.60965 LUMO: 2.33474 factor:1 | 1 (-0.72350) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62970 HOMO: -6.72665 LUMO: 2.25855 factor:1 | 1 (-0.54455) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.36270 HOMO: -6.27495 LUMO: 2.04358 factor:1 | 1 (-0.27756) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.38619 HOMO: -6.17426 LUMO: 1.45853 factor:1 | 1 (-0.30104) | -1 | -1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89670 HOMO: -7.21374 LUMO: 2.33474 factor:1 | 1 (-0.81155) | 1 | 1 |
| G: -6694.71945 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.36447 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-0.27932) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.15551 HOMO: -6.80829 LUMO: 0.17960 factor:1 | 1 (-1.07036) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.43410 HOMO: -7.19469 LUMO: 1.60819 factor:1 | 1 (-0.34896) | 1 | 1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.75460 HOMO: -6.78652 LUMO: 0.53334 factor:1 | 1 (-0.66945) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.09850 HOMO: -6.70489 LUMO: 0.74559 factor:1 | 1 (-1.01335) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.34879 HOMO: -6.72393 LUMO: 0.88981 factor:1 | 1 (-1.26364) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52140 HOMO: -4.54430 LUMO: -0.90614 factor:1 | 1 (-0.43625) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.36531 HOMO: -6.83006 LUMO: 0.47348 factor:1 | 1 (-0.28017) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.42842 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-0.34327) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.52971 HOMO: -6.62053 LUMO: 0.74559 factor:1 | -1 (0.55544) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36887 HOMO: -6.79196 LUMO: 1.80139 factor:1 | 1 (-1.28372) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64121 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-0.55606) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20963 HOMO: -6.74026 LUMO: 0.95784 factor:1 | 1 (-1.12448) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27998 HOMO: -7.34707 LUMO: 0.40001 factor:1 | 1 (-0.19483) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91847 HOMO: -6.19875 LUMO: -0.88709 factor:1 | 1 (-0.83332) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.77797 HOMO: -6.48719 LUMO: -0.14694 factor:1 | 1 (-1.69282) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.40737 HOMO: -6.73482 LUMO: -0.01633 factor:1 | 1 (-2.32222) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.15749 HOMO: -7.05591 LUMO: -0.20136 factor:1 | 1 (-1.07235) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.62558 HOMO: -6.38651 LUMO: -2.07895 factor:1 | 1 (-1.54044) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.41448 HOMO: -6.85455 LUMO: -1.03403 factor:1 | 1 (-1.32933) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.48097 HOMO: -6.72121 LUMO: -0.99322 factor:1 | 1 (-2.39583) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.84379 HOMO: -6.53890 LUMO: -0.10885 factor:1 | 1 (-1.75864) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.48689 HOMO: -6.68312 LUMO: 0.21225 factor:1 | 1 (-1.40174) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.99975 HOMO: -6.68040 LUMO: 0.21225 factor:1 | 1 (-0.91460) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46333 HOMO: -6.76475 LUMO: -0.64491 factor:1 | 1 (-0.37818) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.91280 HOMO: -6.48175 LUMO: 0.41633 factor:1 | 1 (-1.82765) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11510 HOMO: -6.42733 LUMO: 0.16599 factor:1 | 1 (-1.02995) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.63297 HOMO: -6.66679 LUMO: 0.77825 factor:1 | 1 (-2.54783) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.93868 HOMO: -6.75931 LUMO: -0.73471 factor:1 | 1 (-1.85353) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.52000 HOMO: -6.53617 LUMO: 0.38096 factor:1 | 1 (-1.43486) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.72120 HOMO: -6.34297 LUMO: 0.35375 factor:1 | 1 (-1.63606) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.18657 HOMO: -7.11850 LUMO: -0.03265 factor:1 | 1 (-2.10143) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.55840 HOMO: -5.21914 LUMO: 1.29798 factor:1 | 1 (-1.47325) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.79132 HOMO: -7.09129 LUMO: -0.66668 factor:1 | 1 (-2.70617) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.84552 HOMO: -6.96884 LUMO: -0.31021 factor:1 | 1 (-2.76038) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.38163 HOMO: -6.51713 LUMO: -0.59865 factor:1 | 1 (-1.29649) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.66313 HOMO: -6.69400 LUMO: -0.07075 factor:1 | 1 (-1.57799) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.94981 HOMO: -5.28173 LUMO: 1.17281 factor:1 | 1 (-1.86466) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.21796 HOMO: -6.54434 LUMO: 0.32109 factor:1 | 1 (-1.13281) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.03471 HOMO: -6.79740 LUMO: -0.24762 factor:1 | 1 (-1.94956) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36177 HOMO: -6.91986 LUMO: -0.14694 factor:1 | 1 (-1.27662) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.97749 HOMO: -6.75114 LUMO: 0.18504 factor:1 | 1 (-0.89234) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.08554 HOMO: -6.74842 LUMO: 0.69389 factor:1 | 1 (-2.00039) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.09860 HOMO: -7.01782 LUMO: 0.56600 factor:1 | 1 (-2.01345) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.44950 HOMO: -6.47359 LUMO: -0.56600 factor:1 | 1 (-1.36435) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01771 HOMO: -6.63686 LUMO: -0.55783 factor:1 | 1 (-0.93256) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.48778 HOMO: -4.13885 LUMO: -2.05446 factor:1 | 1 (-2.40263) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.41771 HOMO: -6.34570 LUMO: 0.19864 factor:1 | 1 (-1.33257) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.12744 HOMO: -6.47903 LUMO: 0.24762 factor:1 | 1 (-2.04230) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.29902 HOMO: -6.15249 LUMO: 0.32109 factor:1 | 1 (-1.21387) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.32243 HOMO: -6.84366 LUMO: 0.29116 factor:1 | 1 (-0.23728) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36653 HOMO: -6.34297 LUMO: 0.19864 factor:1 | 1 (-1.28138) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.23562 HOMO: -6.51168 LUMO: 0.30749 factor:1 | 1 (-0.15048) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30226 HOMO: -6.79468 LUMO: -0.16599 factor:1 | 1 (-1.21711) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68350 HOMO: -7.24095 LUMO: 0.15238 factor:1 | 1 (-0.59835) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.73081 HOMO: -7.06952 LUMO: -0.34558 factor:1 | 1 (-1.64566) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64360 HOMO: -6.88176 LUMO: 0.02177 factor:1 | 1 (-0.55846) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.55361 HOMO: -6.37291 LUMO: -0.69117 factor:1 | 1 (-1.46846) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.29576 HOMO: -6.83278 LUMO: -0.59049 factor:1 | 1 (-0.21062) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57313 HOMO: -6.57155 LUMO: -0.33470 factor:1 | 1 (-0.48798) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20402 HOMO: -6.89537 LUMO: -0.58504 factor:1 | 1 (-1.11888) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27168 HOMO: -6.57155 LUMO: -0.34831 factor:1 | 1 (-0.18653) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.41332 HOMO: -6.64774 LUMO: -0.95784 factor:1 | 1 (-0.32817) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.96192 HOMO: -6.91713 LUMO: -0.69933 factor:1 | 1 (-1.87677) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61946 HOMO: -6.80557 LUMO: -0.65035 factor:1 | 1 (-1.53431) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50501 HOMO: -7.26544 LUMO: -0.79729 factor:1 | 1 (-1.41986) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.71266 HOMO: -6.69128 LUMO: -0.16871 factor:1 | 1 (-1.62751) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20000 HOMO: -6.88448 LUMO: 0.13061 factor:1 | 1 (-1.11485) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.15173 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-0.06659) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.38362 HOMO: -6.56067 LUMO: 0.17687 factor:1 | 1 (-1.29847) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.41356 HOMO: -6.70216 LUMO: 0.25034 factor:1 | 1 (-0.32841) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17902 HOMO: -6.51713 LUMO: -0.78369 factor:1 | 1 (-1.09387) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.55212 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-0.46697) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64679 HOMO: -6.22052 LUMO: -0.83811 factor:1 | 1 (-0.56164) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.97625 HOMO: -6.51168 LUMO: -0.76464 factor:1 | -1 (0.10890) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.78108 HOMO: -7.14571 LUMO: -0.80274 factor:1 | 1 (-0.69593) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.83139 HOMO: -6.66679 LUMO: -0.88709 factor:1 | 1 (-0.74625) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.18915 HOMO: -6.76203 LUMO: -1.43948 factor:1 | 1 (-0.10400) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68897 HOMO: -6.57427 LUMO: -1.62996 factor:1 | 1 (-0.60382) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.48445 HOMO: -5.05043 LUMO: 1.24900 factor:1 | 1 (-0.39930) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.82630 HOMO: -6.53345 LUMO: 0.23130 factor:1 | 1 (-0.74116) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85049 HOMO: -7.18381 LUMO: -0.22585 factor:1 | 1 (-0.76535) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60619 HOMO: -7.00965 LUMO: -1.79595 factor:1 | 1 (-0.52104) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.96493 HOMO: -6.08174 LUMO: -0.82995 factor:1 | -1 (0.12022) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64513 HOMO: -6.42189 LUMO: -0.84355 factor:1 | 1 (-0.55998) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91517 HOMO: -6.53890 LUMO: 0.60409 factor:1 | 1 (-0.83003) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77659 HOMO: -6.62869 LUMO: 0.43810 factor:1 | 1 (-0.69144) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.22588 HOMO: -6.68312 LUMO: 0.64491 factor:1 | 1 (-0.14074) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76018 HOMO: -6.42189 LUMO: 1.51295 factor:1 | 1 (-0.67503) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69691 HOMO: -6.17971 LUMO: 1.67622 factor:1 | 1 (-0.61177) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50779 HOMO: -6.79196 LUMO: 1.36873 factor:1 | 1 (-0.42265) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.78617 HOMO: -7.38517 LUMO: 0.56328 factor:1 | 1 (-0.70102) | 1 | 1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85038 HOMO: -7.56204 LUMO: 0.71566 factor:1 | 1 (-0.76524) | 1 | 1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.10897 HOMO: -6.45726 LUMO: -1.91840 factor:1 | 1 (-2.02382) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23409 HOMO: -6.13073 LUMO: -0.97417 factor:1 | 1 (-1.14895) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.62047 HOMO: -6.50352 LUMO: -0.69661 factor:1 | 1 (-1.53532) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.74325 HOMO: -6.76747 LUMO: -1.71976 factor:1 | 1 (-0.65811) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.66594 HOMO: -6.48447 LUMO: -0.89525 factor:1 | 1 (-1.58079) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57038 HOMO: -7.11850 LUMO: -0.71566 factor:1 | 1 (-0.48523) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.90790 HOMO: -6.80285 LUMO: -0.49253 factor:1 | 1 (-1.82275) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01553 HOMO: -6.80557 LUMO: -0.88165 factor:1 | 1 (-0.93038) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.80085 HOMO: -6.94162 LUMO: -0.08980 factor:1 | 1 (-1.71571) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80086 HOMO: -6.97972 LUMO: -0.29388 factor:1 | 1 (-0.71571) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50333 HOMO: -6.75114 LUMO: 0.04626 factor:1 | 1 (-0.41818) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.71781 HOMO: -7.15932 LUMO: 0.68845 factor:1 | 1 (-0.63266) | 1 | 1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.78820 HOMO: -7.36612 LUMO: 0.63675 factor:1 | 1 (-1.70305) | 1 | 1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.29681 HOMO: -7.02598 LUMO: -0.66124 factor:1 | 1 (-1.21167) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50899 HOMO: -6.89264 LUMO: -0.54967 factor:1 | 1 (-0.42384) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.03004 HOMO: -6.97700 LUMO: 0.27756 factor:1 | -1 (0.05510) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59835 HOMO: -6.60965 LUMO: 0.08163 factor:1 | 1 (-0.51321) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.52210 HOMO: -6.70761 LUMO: 0.40001 factor:1 | 1 (-1.43695) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.37761 HOMO: -6.69128 LUMO: 0.23674 factor:1 | 1 (-0.29247) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.96747 HOMO: -6.69128 LUMO: -0.69933 factor:1 | 1 (-1.88232) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.56051 HOMO: -6.18515 LUMO: -0.85988 factor:1 | 1 (-2.47537) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.41821 HOMO: -6.86815 LUMO: -1.90208 factor:1 | 1 (-0.33307) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.71622 HOMO: -6.37563 LUMO: -1.74697 factor:1 | 1 (-1.63108) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.48064 HOMO: -6.75659 LUMO: 0.36463 factor:1 | -1 (0.60450) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.72281 HOMO: -6.91441 LUMO: -0.88981 factor:1 | 1 (-1.63766) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.93552 HOMO: -6.71305 LUMO: -0.29933 factor:1 | 1 (-1.85037) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64282 HOMO: -6.91441 LUMO: -1.04492 factor:1 | 1 (-0.55767) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60178 HOMO: -6.05453 LUMO: -0.83539 factor:1 | 1 (-0.51664) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62126 HOMO: -7.35252 LUMO: -0.45715 factor:1 | 1 (-0.53612) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.51776 HOMO: -6.41644 LUMO: -0.97417 factor:1 | 1 (-2.43262) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61864 HOMO: -6.78924 LUMO: 0.36735 factor:1 | 1 (-1.53350) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.21066 HOMO: -6.74298 LUMO: 0.51974 factor:1 | 1 (-1.12552) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.67475 HOMO: -6.48992 LUMO: 1.44765 factor:1 | 1 (-1.58961) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.24073 HOMO: -6.12528 LUMO: 1.57826 factor:1 | 1 (-1.15559) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.85606 HOMO: -6.62325 LUMO: 1.57826 factor:1 | 1 (-1.77092) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.44547 HOMO: -6.19875 LUMO: 1.29798 factor:1 | 1 (-1.36032) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.64594 HOMO: -6.74570 LUMO: 1.52112 factor:1 | 1 (-1.56079) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.26122 HOMO: -6.84094 LUMO: 1.48574 factor:1 | 1 (-1.17608) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.43488 HOMO: -6.85183 LUMO: 0.33470 factor:1 | 1 (-1.34974) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45326 HOMO: -6.51168 LUMO: 0.48164 factor:1 | 1 (-0.36812) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27641 HOMO: -6.25046 LUMO: 0.75648 factor:1 | 1 (-0.19127) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70116 HOMO: -6.65591 LUMO: 0.32109 factor:1 | 1 (-0.61601) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59963 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-0.51449) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59068 HOMO: -6.75114 LUMO: 0.73471 factor:1 | 1 (-0.50553) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.92835 HOMO: -6.50624 LUMO: 0.59321 factor:1 | -1 (0.15679) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.65019 HOMO: -6.39740 LUMO: 0.83267 factor:1 | 1 (-0.56504) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89858 HOMO: -6.44094 LUMO: 0.65579 factor:1 | 1 (-0.81343) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.44415 HOMO: -6.52257 LUMO: 0.05714 factor:1 | 1 (-0.35900) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.33788 HOMO: -7.10217 LUMO: 0.49797 factor:1 | 1 (-1.25273) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.51021 HOMO: -6.83006 LUMO: 0.55783 factor:1 | 1 (-0.42507) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.22642 HOMO: -6.99333 LUMO: -0.79457 factor:1 | 1 (-1.14127) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.72404 HOMO: -6.64230 LUMO: 0.32382 factor:1 | 1 (-0.63890) | -1 | -1 |
| G: -6694.71945 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50015 HOMO: -6.90897 LUMO: 0.30749 factor:1 | 1 (-0.41500) | -1 | -1 |
| G: -6694.71945 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.26107 HOMO: -7.09129 LUMO: 1.33336 factor:1 | 1 (-0.17592) | 1 | 1 |
| G: -6695.41329 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.63887 HOMO: -6.66951 LUMO: 1.34424 factor:1 | -1 (0.14011) | -1 | -1 |
| G: -6695.41329 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.02017 HOMO: -7.02870 LUMO: 1.48574 factor:1 | -1 (1.75881) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.96118 HOMO: -7.26544 LUMO: 0.32926 factor:1 | -1 (1.81780) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.84865 HOMO: -6.56067 LUMO: -0.45987 factor:1 | -1 (0.93033) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.03949 HOMO: -6.54434 LUMO: -0.28300 factor:1 | -1 (0.73950) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60491 HOMO: -7.19469 LUMO: 0.54695 factor:1 | -1 (0.17407) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.94545 HOMO: -6.47359 LUMO: -0.22041 factor:1 | -1 (1.83353) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.22447 HOMO: -6.80013 LUMO: 2.08167 factor:1 | -1 (0.55451) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.35449 HOMO: -6.23957 LUMO: 1.67894 factor:1 | -1 (1.42449) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.47621 HOMO: -6.75114 LUMO: -0.62858 factor:1 | -1 (1.30277) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.99465 HOMO: -6.79468 LUMO: -0.64491 factor:1 | -1 (1.78433) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.57031 HOMO: -6.84911 LUMO: -0.69661 factor:1 | -1 (1.20868) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.71790 HOMO: -7.54028 LUMO: 0.25851 factor:1 | -1 (1.06108) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.33816 HOMO: -6.92802 LUMO: -0.71022 factor:1 | -1 (0.44082) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.89367 HOMO: -6.72665 LUMO: -0.46804 factor:1 | -1 (1.88531) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.38072 HOMO: -6.63686 LUMO: -0.23674 factor:1 | -1 (1.39826) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.69654 HOMO: -7.21102 LUMO: 0.54423 factor:1 | -1 (1.08244) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.62337 HOMO: -6.63414 LUMO: -0.25034 factor:1 | -1 (1.15561) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.14289 HOMO: -6.70761 LUMO: -0.31837 factor:1 | -1 (0.63609) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.51496 HOMO: -6.57155 LUMO: 1.76874 factor:1 | -1 (1.26402) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.77865 HOMO: -6.84366 LUMO: 2.04358 factor:1 | -1 (2.00034) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.98790 HOMO: -6.60420 LUMO: 1.80139 factor:1 | -1 (1.79108) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.61189 HOMO: -7.03686 LUMO: 2.21229 factor:1 | -1 (1.16710) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.86825 HOMO: -6.77564 LUMO: 1.97555 factor:1 | -1 (1.91073) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.98287 HOMO: -6.40012 LUMO: 2.17691 factor:1 | -1 (1.79611) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.49322 HOMO: -6.80013 LUMO: 2.25582 factor:1 | -1 (1.28577) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.48845 HOMO: -6.74298 LUMO: 2.31569 factor:1 | -1 (1.29053) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.41879 HOMO: -6.68856 LUMO: 1.85854 factor:1 | -1 (1.36019) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.49959 HOMO: -6.17971 LUMO: 1.52928 factor:1 | -1 (2.27939) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.58626 HOMO: -6.54162 LUMO: 1.91840 factor:1 | -1 (2.19272) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.73620 HOMO: -6.80013 LUMO: -0.55511 factor:1 | -1 (2.04279) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.77799 HOMO: -7.46953 LUMO: 0.28572 factor:1 | -1 (2.00099) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.43230 HOMO: -6.61781 LUMO: -0.54967 factor:1 | -1 (2.34668) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.84327 HOMO: -6.56339 LUMO: -0.47892 factor:1 | -1 (1.93571) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.37588 HOMO: -6.65591 LUMO: -0.25307 factor:1 | -1 (1.40310) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.43419 HOMO: -6.62869 LUMO: -0.23402 factor:1 | -1 (1.34479) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.51915 HOMO: -6.58243 LUMO: -0.19048 factor:1 | -1 (1.25983) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.23035 HOMO: -7.27632 LUMO: 0.52790 factor:1 | -1 (1.54863) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.81380 HOMO: -7.21102 LUMO: 0.57688 factor:1 | -1 (1.96518) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.45841 HOMO: -6.72393 LUMO: -0.53879 factor:1 | -1 (1.32057) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.69975 HOMO: -7.42054 LUMO: -0.99322 factor:1 | -1 (1.07923) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.45477 HOMO: -6.88992 LUMO: -0.71838 factor:1 | -1 (1.32421) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.60867 HOMO: -6.88176 LUMO: -0.61226 factor:1 | -1 (1.17031) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.27404 HOMO: -7.36340 LUMO: -1.04492 factor:1 | -1 (2.50494) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.54278 HOMO: -6.65863 LUMO: -0.41906 factor:1 | -1 (2.23620) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.69641 HOMO: -7.15115 LUMO: -0.66396 factor:1 | -1 (2.08257) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.84360 HOMO: -7.10489 LUMO: -0.64491 factor:1 | -1 (1.93538) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.70558 HOMO: -7.20285 LUMO: 0.47892 factor:1 | -1 (2.07340) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.40652 HOMO: -6.55794 LUMO: -0.28844 factor:1 | -1 (1.37246) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.87470 HOMO: -7.19197 LUMO: -0.69661 factor:1 | -1 (1.90428) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.00730 HOMO: -6.56883 LUMO: -0.32926 factor:1 | -1 (1.77168) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.38837 HOMO: -6.70761 LUMO: 1.95650 factor:1 | -1 (1.39061) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.34170 HOMO: -6.60420 LUMO: 1.80684 factor:1 | -1 (1.43728) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.42769 HOMO: -6.84094 LUMO: 1.64085 factor:1 | -1 (1.35129) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.60675 HOMO: -6.69128 LUMO: 1.90208 factor:1 | -1 (2.17223) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.81437 HOMO: -6.75387 LUMO: 1.70343 factor:1 | -1 (1.96461) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.77655 HOMO: -7.07496 LUMO: 2.10072 factor:1 | -1 (2.00243) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.05734 HOMO: -6.99877 LUMO: 2.24494 factor:1 | -1 (0.72165) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.11902 HOMO: -6.63414 LUMO: 2.17691 factor:1 | -1 (0.65996) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57136 HOMO: -6.44638 LUMO: 1.78235 factor:1 | -1 (0.20762) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.43413 HOMO: -6.87632 LUMO: 1.84221 factor:1 | -1 (0.34485) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70157 HOMO: -6.85183 LUMO: 1.68711 factor:1 | -1 (0.07742) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.90530 HOMO: -6.96339 LUMO: 2.26671 factor:1 | 1 (-0.12632) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61590 HOMO: -6.63141 LUMO: 1.96738 factor:1 | 1 (-0.83691) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.32256 HOMO: -6.37019 LUMO: 2.23133 factor:1 | 1 (-0.54357) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.32286 HOMO: -7.11034 LUMO: 2.32385 factor:1 | -1 (0.45612) | 1 | 1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.32844 HOMO: -6.91986 LUMO: 1.65445 factor:1 | -1 (0.45054) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14242 HOMO: -7.12938 LUMO: 2.28304 factor:1 | 1 (-0.36344) | 1 | 1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.99322 HOMO: -6.54978 LUMO: 1.92112 factor:1 | 1 (-0.21424) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.22207 HOMO: -6.83006 LUMO: 2.48712 factor:1 | -1 (0.55691) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.33846 HOMO: -6.97972 LUMO: 1.96738 factor:1 | -1 (0.44053) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.19110 HOMO: -6.69944 LUMO: 2.06262 factor:1 | 1 (-0.41212) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17722 HOMO: -6.76747 LUMO: 2.10888 factor:1 | 1 (-0.39824) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.02557 HOMO: -6.91169 LUMO: 2.06534 factor:1 | 1 (-0.24659) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.26425 HOMO: -7.03414 LUMO: 1.93473 factor:1 | -1 (0.51473) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.19676 HOMO: -7.03142 LUMO: 2.52250 factor:1 | 1 (-0.41778) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.94447 HOMO: -6.34025 LUMO: 2.61229 factor:1 | 1 (-1.16549) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.17552 HOMO: -6.98788 LUMO: 2.28304 factor:1 | 1 (-1.39654) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.06907 HOMO: -6.97700 LUMO: 2.53882 factor:1 | 1 (-1.29009) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.90021 HOMO: -6.58788 LUMO: 1.94289 factor:1 | 1 (-0.12123) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01561 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-0.23663) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.39316 HOMO: -6.55250 LUMO: 1.82861 factor:1 | 1 (-1.61418) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.05207 HOMO: -6.45998 LUMO: 1.75786 factor:1 | 1 (-1.27308) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.34079 HOMO: -6.78924 LUMO: 2.33746 factor:1 | 1 (-0.56181) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.32166 HOMO: -6.85727 LUMO: 1.76058 factor:1 | 1 (-0.54268) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.29031 HOMO: -6.70489 LUMO: 1.84493 factor:1 | 1 (-0.51133) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.64528 HOMO: -6.71305 LUMO: 1.53472 factor:1 | 1 (-0.86630) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.64387 HOMO: -6.76747 LUMO: 1.48846 factor:1 | 1 (-0.86489) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.63356 HOMO: -6.69128 LUMO: 1.95922 factor:1 | 1 (-0.85457) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.56169 HOMO: -6.67495 LUMO: 2.05446 factor:1 | 1 (-0.78271) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.75075 HOMO: -6.63686 LUMO: 2.25310 factor:1 | 1 (-0.97177) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.72543 HOMO: -6.63958 LUMO: 2.14154 factor:1 | -1 (0.05355) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.08680 HOMO: -6.62597 LUMO: 2.01908 factor:1 | 1 (-0.30782) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.07806 HOMO: -7.07768 LUMO: 2.14154 factor:1 | 1 (-0.29908) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61802 HOMO: -6.19603 LUMO: 2.01092 factor:1 | 1 (-0.83904) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.39189 HOMO: -6.65046 LUMO: 2.15786 factor:1 | 1 (-0.61291) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.46705 HOMO: -6.92258 LUMO: 2.31841 factor:1 | 1 (-0.68807) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50338 HOMO: -6.90081 LUMO: 2.19324 factor:1 | 1 (-0.72439) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.37259 HOMO: -6.85455 LUMO: 1.95650 factor:1 | -1 (1.40639) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.34846 HOMO: -6.57699 LUMO: 1.76058 factor:1 | 1 (-0.56948) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.27950 HOMO: -6.90625 LUMO: 1.97555 factor:1 | 1 (-1.50052) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.08262 HOMO: -6.97428 LUMO: 1.92929 factor:1 | 1 (-1.30364) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30188 HOMO: -6.61781 LUMO: -0.41906 factor:1 | 1 (-0.52289) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.99265 HOMO: -6.62869 LUMO: -0.81906 factor:1 | 1 (-0.21366) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85828 HOMO: -7.01237 LUMO: 2.00548 factor:1 | 1 (-0.07929) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.70827 HOMO: -6.85727 LUMO: 2.17691 factor:1 | -1 (1.07071) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.33518 HOMO: -6.71849 LUMO: 1.58914 factor:1 | 1 (-0.55620) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.51894 HOMO: -7.52395 LUMO: 0.27211 factor:1 | 1 (-0.73996) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.62153 HOMO: -6.96611 LUMO: -0.72654 factor:1 | 1 (-0.84255) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.23651 HOMO: -6.89537 LUMO: -0.68028 factor:1 | 1 (-1.45752) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.95772 HOMO: -6.84911 LUMO: -0.58504 factor:1 | 1 (-1.17874) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.34931 HOMO: -6.79196 LUMO: -0.55783 factor:1 | 1 (-0.57032) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36041 HOMO: -6.67767 LUMO: 1.79323 factor:1 | 1 (-0.58143) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46777 HOMO: -6.54434 LUMO: 1.91024 factor:1 | -1 (0.31122) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.24041 HOMO: -6.62869 LUMO: 1.69799 factor:1 | 1 (-0.46142) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14253 HOMO: -6.72393 LUMO: 2.12249 factor:1 | 1 (-0.36354) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50823 HOMO: -6.66407 LUMO: 2.05990 factor:1 | -1 (0.27075) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.40899 HOMO: -7.00149 LUMO: 1.82044 factor:1 | -1 (0.36999) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.57270 HOMO: -7.12122 LUMO: 2.16058 factor:1 | 1 (-1.79372) | 1 | 1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.97362 HOMO: -6.63141 LUMO: 2.21229 factor:1 | 1 (-1.19463) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.83024 HOMO: -6.37835 LUMO: 2.32113 factor:1 | 1 (-1.05126) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.81624 HOMO: -6.99605 LUMO: 2.00548 factor:1 | 1 (-2.03726) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.40586 HOMO: -6.85999 LUMO: 2.39460 factor:1 | -1 (0.37312) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20250 HOMO: -6.85727 LUMO: 2.48712 factor:1 | 1 (-0.42352) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60290 HOMO: -7.04231 LUMO: 2.40277 factor:1 | -1 (0.17608) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.39741 HOMO: -6.60692 LUMO: 2.26671 factor:1 | 1 (-0.61843) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.28195 HOMO: -6.67495 LUMO: 2.14698 factor:1 | 1 (-1.50297) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.46345 HOMO: -6.73210 LUMO: 2.06807 factor:1 | 1 (-1.68447) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.54953 HOMO: -7.20013 LUMO: 2.02181 factor:1 | 1 (-0.77054) | 1 | 1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.28562 HOMO: -7.18653 LUMO: 2.29936 factor:1 | 1 (-1.50664) | 1 | 1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.60164 HOMO: -6.92802 LUMO: 2.36195 factor:1 | 1 (-0.82265) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.41758 HOMO: -6.89537 LUMO: 1.78779 factor:1 | 1 (-0.63860) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.19841 HOMO: -6.96067 LUMO: 2.31297 factor:1 | 1 (-1.41943) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.83965 HOMO: -6.91441 LUMO: 2.50345 factor:1 | 1 (-1.06067) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.54482 HOMO: -7.17292 LUMO: 2.12521 factor:1 | 1 (-0.76584) | 1 | 1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.94965 HOMO: -6.93618 LUMO: 2.35106 factor:1 | 1 (-0.17067) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.93248 HOMO: -6.75931 LUMO: 1.61908 factor:1 | 1 (-0.15350) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.04886 HOMO: -6.35930 LUMO: 1.23540 factor:1 | 1 (-0.26988) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05474 HOMO: -6.17971 LUMO: 1.84493 factor:1 | 1 (-0.27576) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.93931 HOMO: -6.72665 LUMO: 2.61229 factor:1 | 1 (-0.16033) | -1 | -1 |
| G: -6695.41329 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.19093 HOMO: -6.62869 LUMO: 2.28304 factor:1 | 1 (-1.41194) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.51129 HOMO: -6.58243 LUMO: 0.28028 factor:1 | 1 (-0.73231) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.51423 HOMO: -6.79468 LUMO: 0.14966 factor:1 | 1 (-0.73525) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69974 HOMO: -6.63141 LUMO: 0.31021 factor:1 | -1 (0.07924) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.04418 HOMO: -6.81101 LUMO: 0.13878 factor:1 | 1 (-1.26519) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30291 HOMO: -6.72665 LUMO: 0.65579 factor:1 | 1 (-0.52393) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.92093 HOMO: -6.53073 LUMO: 0.91430 factor:1 | 1 (-1.14195) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.20886 HOMO: -7.19197 LUMO: 1.62996 factor:1 | 1 (-1.42988) | 1 | 1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.36843 HOMO: -6.69400 LUMO: 0.84627 factor:1 | 1 (-1.58944) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.76123 HOMO: -6.76475 LUMO: 0.51974 factor:1 | 1 (-0.98225) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87215 HOMO: -6.67767 LUMO: 0.52246 factor:1 | 1 (-0.09317) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.87800 HOMO: -6.73210 LUMO: 0.94424 factor:1 | 1 (-1.09901) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.79724 HOMO: -6.97972 LUMO: 0.60409 factor:1 | 1 (-0.01826) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.73715 HOMO: -7.38517 LUMO: 0.73743 factor:1 | 1 (-0.95817) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.76556 HOMO: -6.48992 LUMO: 1.08301 factor:1 | 1 (-0.98658) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.84975 HOMO: -7.18381 LUMO: 1.61908 factor:1 | 1 (-1.07077) | 1 | 1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69588 HOMO: -6.74842 LUMO: 0.57960 factor:1 | -1 (0.08310) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.76787 HOMO: -6.67495 LUMO: 0.77280 factor:1 | 1 (-0.98889) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.51984 HOMO: -6.74570 LUMO: 0.77280 factor:1 | 1 (-0.74086) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.53419 HOMO: -6.73754 LUMO: 0.86804 factor:1 | -1 (0.24479) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.00905 HOMO: -6.66135 LUMO: 0.94424 factor:1 | 1 (-0.23007) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.00541 HOMO: -6.44638 LUMO: 1.00138 factor:1 | 1 (-0.22643) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.38572 HOMO: -6.65591 LUMO: 1.02043 factor:1 | -1 (0.39326) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.14954 HOMO: -7.17564 LUMO: 0.50069 factor:1 | -1 (1.62945) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.02753 HOMO: -6.59332 LUMO: 0.79457 factor:1 | 1 (-0.24855) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88380 HOMO: -6.76747 LUMO: 1.73881 factor:1 | 1 (-0.10482) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.32526 HOMO: -7.00421 LUMO: 1.07485 factor:1 | -1 (0.45372) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01548 HOMO: -6.94979 LUMO: 1.67894 factor:1 | 1 (-0.23649) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.78048 HOMO: -6.66135 LUMO: 0.47076 factor:1 | 1 (-0.00150) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76238 HOMO: -6.74298 LUMO: 1.85037 factor:1 | -1 (0.01660) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.13011 HOMO: -6.65318 LUMO: 0.95240 factor:1 | 1 (-1.35113) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.24772 HOMO: -6.63958 LUMO: 0.78097 factor:1 | 1 (-0.46874) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.04143 HOMO: -6.11712 LUMO: 0.40001 factor:1 | 1 (-1.26245) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.98486 HOMO: -7.08312 LUMO: 0.92519 factor:1 | 1 (-0.20588) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91267 HOMO: -6.96067 LUMO: 0.54695 factor:1 | 1 (-0.13369) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.68166 HOMO: -6.74026 LUMO: 0.60137 factor:1 | 1 (-1.90267) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.12992 HOMO: -6.74298 LUMO: 0.59593 factor:1 | 1 (-1.35094) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.64881 HOMO: -6.93074 LUMO: 0.60681 factor:1 | 1 (-1.86983) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.10682 HOMO: -6.41644 LUMO: 0.35919 factor:1 | 1 (-1.32783) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.58945 HOMO: -6.41917 LUMO: 1.73064 factor:1 | 1 (-0.81046) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.58980 HOMO: -4.64226 LUMO: -0.87893 factor:1 | 1 (-0.81082) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.08772 HOMO: -6.59604 LUMO: 0.90342 factor:1 | 1 (-0.30874) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.69851 HOMO: -6.79468 LUMO: 0.50069 factor:1 | 1 (-0.91953) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.86062 HOMO: -7.04503 LUMO: 0.52518 factor:1 | 1 (-0.08163) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.84051 HOMO: -6.69400 LUMO: 0.54423 factor:1 | 1 (-0.06152) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.09793 HOMO: -6.51713 LUMO: 0.95240 factor:1 | 1 (-0.31894) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.97599 HOMO: -6.88176 LUMO: 1.79323 factor:1 | 1 (-0.19701) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89485 HOMO: -6.71849 LUMO: 0.28844 factor:1 | 1 (-0.11587) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06778 HOMO: -6.94979 LUMO: 0.51974 factor:1 | 1 (-0.28879) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01877 HOMO: -6.76203 LUMO: 0.94151 factor:1 | 1 (-0.23979) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76984 HOMO: -6.91169 LUMO: 0.89525 factor:1 | -1 (0.00914) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.92092 HOMO: -6.83006 LUMO: 0.89253 factor:1 | 1 (-0.14193) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.63718 HOMO: -7.08857 LUMO: 0.60409 factor:1 | -1 (0.14180) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77204 HOMO: -6.91713 LUMO: 1.76330 factor:1 | -1 (0.00694) | -1 | -1 |
| G: -6695.41329 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.35545 HOMO: -6.47359 LUMO: 1.56193 factor:1 | -1 (1.42354) | -1 | -1 |
| G: -6695.41329 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.85269 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-1.07371) | -1 | -1 |
| G: -6695.41329 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.87609 HOMO: -7.03686 LUMO: 1.97283 factor:1 | 1 (-1.09711) | -1 | -1 |
| G: -6695.41329 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.77575 HOMO: -7.00965 LUMO: 1.64629 factor:1 | -1 (1.00323) | -1 | -1 |
| G: -6695.41329 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.20256 HOMO: -7.06952 LUMO: 1.67622 factor:1 | -1 (0.57642) | 1 | -1 |
| G: -6695.41329 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.25694 HOMO: -6.80557 LUMO: 1.70615 factor:1 | 1 (-1.47796) | -1 | -1 |
| G: -6695.41329 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.35542 HOMO: -6.80829 LUMO: 1.71704 factor:1 | 1 (-1.57644) | -1 | -1 |
| G: -6695.41329 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.85875 HOMO: -7.26544 LUMO: 1.89935 factor:1 | 1 (-2.07977) | 1 | -1 |
| G: -6695.41329 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.56982 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-1.79084) | -1 | -1 |
| G: -6695.41329 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.27461 HOMO: -7.03686 LUMO: 1.97283 factor:1 | 1 (-0.49563) | -1 | -1 |
| G: -6695.41329 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88415 HOMO: -7.00965 LUMO: 1.64629 factor:1 | 1 (-0.10517) | -1 | -1 |
| G: -6695.41329 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.83476 HOMO: -7.06952 LUMO: 1.67622 factor:1 | 1 (-0.05578) | -1 | -1 |
| G: -6695.41329 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.31880 HOMO: -6.80557 LUMO: 1.70615 factor:1 | 1 (-0.53982) | -1 | -1 |
| G: -6695.41329 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87308 HOMO: -6.80829 LUMO: 1.71704 factor:1 | 1 (-0.09410) | -1 | -1 |
| G: -6695.41329 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81719 HOMO: -7.26544 LUMO: 1.89935 factor:1 | 1 (-0.03820) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.95030 HOMO: -7.00149 LUMO: 1.75241 factor:1 | 1 (-0.17132) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61810 HOMO: -6.91169 LUMO: 2.07079 factor:1 | 1 (-0.83912) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.74714 HOMO: -7.11034 LUMO: 1.76330 factor:1 | -1 (0.03184) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.44647 HOMO: -6.87360 LUMO: 2.02725 factor:1 | 1 (-1.66749) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.30192 HOMO: -7.08584 LUMO: 1.82044 factor:1 | 1 (-1.52294) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.81203 HOMO: -6.90625 LUMO: 1.68166 factor:1 | 1 (-1.03305) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96301 HOMO: -6.71577 LUMO: 1.93201 factor:1 | 1 (-0.18403) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.86390 HOMO: -6.99605 LUMO: 2.08439 factor:1 | 1 (-1.08492) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.20078 HOMO: -7.02326 LUMO: 1.97010 factor:1 | 1 (-1.42179) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.52580 HOMO: -6.99877 LUMO: 2.15514 factor:1 | 1 (-0.74682) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.54095 HOMO: -6.75387 LUMO: 1.95106 factor:1 | 1 (-0.76197) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.91030 HOMO: -7.10761 LUMO: 2.06262 factor:1 | 1 (-1.13131) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.91674 HOMO: -7.03142 LUMO: 1.91568 factor:1 | 1 (-1.13776) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.98486 HOMO: -6.98788 LUMO: 1.98371 factor:1 | 1 (-0.20588) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.29735 HOMO: -6.94707 LUMO: 1.68438 factor:1 | 1 (-1.51837) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.57720 HOMO: -6.88176 LUMO: 2.20684 factor:1 | 1 (-0.79822) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.52457 HOMO: -6.73210 LUMO: 2.18780 factor:1 | 1 (-0.74559) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.86817 HOMO: -6.83822 LUMO: 2.06807 factor:1 | 1 (-1.08919) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.42028 HOMO: -6.78924 LUMO: 2.42181 factor:1 | -1 (0.35870) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.51561 HOMO: -6.94707 LUMO: 1.71704 factor:1 | -1 (1.26337) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.07045 HOMO: -6.85183 LUMO: 1.78779 factor:1 | -1 (0.70853) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.13884 HOMO: -6.98788 LUMO: 1.69799 factor:1 | 1 (-1.35986) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.15300 HOMO: -6.79468 LUMO: 2.04358 factor:1 | 1 (-0.37402) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.02703 HOMO: -6.90081 LUMO: 1.97283 factor:1 | 1 (-1.24805) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.13491 HOMO: -6.79468 LUMO: 2.00820 factor:1 | 1 (-0.35592) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.48446 HOMO: -7.06408 LUMO: 2.29936 factor:1 | 1 (-0.70548) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.61857 HOMO: -6.78924 LUMO: 2.13337 factor:1 | -1 (0.16041) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.75225 HOMO: -6.79468 LUMO: 2.35106 factor:1 | 1 (-0.97327) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.53881 HOMO: -6.82734 LUMO: 2.16603 factor:1 | 1 (-0.75982) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.66946 HOMO: -6.79740 LUMO: 2.36739 factor:1 | -1 (0.10953) | -1 | -1 |
| G: -6695.41329 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.39054 HOMO: -7.14027 LUMO: 2.10888 factor:1 | -1 (0.38844) | -1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.98159 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.20261) | -1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87452 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.09554) | -1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36873 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-0.58975) | -1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80481 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.02582) | -1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60643 HOMO: -6.72121 LUMO: 1.43132 factor:1 | -1 (0.17255) | -1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.65695 HOMO: -6.51168 LUMO: 1.72520 factor:1 | -1 (1.12203) | -1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79799 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-1.01901) | -1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.08130 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.30232) | -1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.63021 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.85123) | -1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.38437 HOMO: -6.82462 LUMO: 1.86670 factor:1 | -1 (1.39461) | -1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.10922 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.33024) | -1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14674 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-0.36776) | -1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.17071 HOMO: -6.84094 LUMO: 1.27349 factor:1 | -1 (1.60827) | -1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.93507 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-0.15608) | 1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23368 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.45470) | 1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17439 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-0.39541) | -1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.16519 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.38621) | 1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.67919 HOMO: -6.68584 LUMO: 1.91296 factor:1 | -1 (2.09979) | -1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57460 HOMO: -7.09129 LUMO: 1.73609 factor:1 | -1 (0.20438) | 1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.61140 HOMO: -7.01237 LUMO: 2.01092 factor:1 | -1 (1.16759) | -1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.90023 HOMO: -6.93618 LUMO: 1.63540 factor:1 | -1 (1.87876) | -1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88843 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.10944) | -1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.19913 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.42014) | -1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.75618 HOMO: -6.76747 LUMO: 1.88303 factor:1 | -1 (0.02280) | -1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.92394 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.14496) | -1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.42717 HOMO: -6.93618 LUMO: 2.19324 factor:1 | -1 (0.35182) | -1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.50350 HOMO: -6.95523 LUMO: 1.80684 factor:1 | -1 (1.27548) | -1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.55722 HOMO: -6.66135 LUMO: 1.72792 factor:1 | -1 (1.22176) | -1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.22442 HOMO: -6.36202 LUMO: 1.89391 factor:1 | -1 (1.55456) | -1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.31417 HOMO: -7.03959 LUMO: 2.06262 factor:1 | -1 (1.46482) | -1 | -1 |
| G: -6695.41329 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52616 HOMO: -7.08584 LUMO: 2.01092 factor:1 | -1 (0.25282) | 1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.67061 HOMO: -6.96067 LUMO: 1.59731 factor:1 | -1 (1.10837) | -1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.37283 HOMO: -6.91169 LUMO: 1.37145 factor:1 | -1 (1.40615) | -1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.92392 HOMO: -6.94707 LUMO: 1.73064 factor:1 | -1 (0.85506) | -1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.71513 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.93615) | -1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05575 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.27677) | -1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.81818 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-1.03920) | -1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.29227 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.51329) | -1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.08797 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.30899) | -1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.19039 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.41141) | -1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.74292 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.96394) | -1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14408 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.36510) | -1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14500 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-0.36602) | -1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80105 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-0.02207) | -1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.92046 HOMO: -7.07768 LUMO: 1.27621 factor:1 | -1 (0.85852) | 1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.03678 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.25780) | 1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81645 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-0.03747) | -1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11678 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.33780) | 1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.27583 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.49685) | -1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11510 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.33612) | 1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.07253 HOMO: -7.01237 LUMO: 2.01092 factor:1 | -1 (1.70645) | -1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.47333 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-0.69435) | -1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.31834 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.53936) | -1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81762 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.03864) | -1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.04264 HOMO: -6.76747 LUMO: 1.88303 factor:1 | -1 (0.73634) | -1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.27992 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.50093) | -1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.02307 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-0.24409) | -1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01436 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.23538) | -1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.10908 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-0.33010) | -1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62080 HOMO: -6.36202 LUMO: 1.89391 factor:1 | -1 (0.15818) | -1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.99608 HOMO: -7.03959 LUMO: 2.06262 factor:1 | -1 (0.78290) | -1 | -1 |
| G: -6695.41329 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.32343 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.54445) | 1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45862 HOMO: -6.96067 LUMO: 1.59731 factor:1 | -1 (0.32036) | -1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23709 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.45810) | -1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57179 HOMO: -6.94707 LUMO: 1.73064 factor:1 | -1 (0.20719) | -1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62692 HOMO: -7.02326 LUMO: 1.41227 factor:1 | -1 (0.15206) | -1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.66762 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.88864) | -1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.33769 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.55870) | -1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.65840 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.87942) | -1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.84625 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.06727) | -1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.51625 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.73727) | -1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79691 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-1.01792) | -1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05637 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.27739) | -1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.95108 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.17210) | -1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.98037 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-0.20139) | -1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.92230 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.14331) | -1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.69157 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.91259) | -1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87253 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-0.09355) | -1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.53285 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.75386) | -1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01246 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.23347) | -1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.58158 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.80260) | -1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.74490 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-0.96592) | -1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.63998 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-0.86100) | -1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.26777 HOMO: -6.98516 LUMO: 1.64629 factor:1 | -1 (1.51121) | -1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.63481 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.85583) | -1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64986 HOMO: -6.76747 LUMO: 1.88303 factor:1 | -1 (0.12912) | -1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06514 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.28615) | -1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.72399 HOMO: -6.93618 LUMO: 2.19324 factor:1 | -1 (0.05499) | -1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11714 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.33816) | -1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.13058 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-0.35160) | -1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96761 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.18863) | -1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06587 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.28689) | -1 | -1 |
| G: -6695.41329 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.28364 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.50466) | -1 | -1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.22283 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-0.44384) | 1 | 1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30511 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.52613) | -1 | -1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.37377 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-0.59479) | 1 | 1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89798 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.11900) | -1 | -1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.44737 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.66839) | -1 | -1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.29942 HOMO: -6.51168 LUMO: 1.72520 factor:1 | -1 (1.47956) | 1 | 1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89858 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.11959) | 1 | 1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52850 HOMO: -6.92802 LUMO: 2.07895 factor:1 | -1 (0.25048) | 1 | 1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.60209 HOMO: -7.02326 LUMO: 1.86398 factor:1 | -1 (1.17689) | 1 | 1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.37032 HOMO: -6.82462 LUMO: 1.86670 factor:1 | -1 (0.40866) | 1 | 1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88788 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.10890) | 1 | 1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.38795 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-0.60896) | 1 | 1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.37668 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-0.59770) | -1 | -1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.67181 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-0.89283) | -1 | -1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85602 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.07704) | -1 | -1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.72486 HOMO: -6.94162 LUMO: 1.64629 factor:1 | -1 (0.05412) | 1 | 1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.78096 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.00198) | 1 | 1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.86829 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.08931) | 1 | 1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.64338 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.86440) | 1 | 1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59332 HOMO: -7.01237 LUMO: 2.01092 factor:1 | -1 (0.18566) | 1 | 1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.65383 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-0.87485) | 1 | 1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.12617 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.34719) | 1 | 1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.99953 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.22055) | 1 | 1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.34129 HOMO: -6.76747 LUMO: 1.88303 factor:1 | -1 (0.43770) | 1 | 1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.00239 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.22341) | 1 | 1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.44245 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-0.66347) | 1 | 1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.46150 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.68252) | 1 | 1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.68420 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-0.90521) | 1 | 1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.42294 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.64396) | -1 | -1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.43369 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.65471) | 1 | 1 |
| G: -6695.41329 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.70158 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.92260) | 1 | 1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.46052 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-0.68154) | 1 | 1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64154 HOMO: -6.91169 LUMO: 1.37145 factor:1 | -1 (0.13744) | -1 | -1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20498 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-0.42599) | 1 | 1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.31916 HOMO: -7.02326 LUMO: 1.41227 factor:1 | -1 (0.45982) | -1 | -1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.65620 HOMO: -6.72121 LUMO: 1.43132 factor:1 | -1 (0.12278) | -1 | -1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.68316 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.90418) | -1 | -1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.87035 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-1.09137) | 1 | 1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81776 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.03878) | 1 | 1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46567 HOMO: -7.02326 LUMO: 1.86398 factor:1 | -1 (0.31331) | 1 | 1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.11546 HOMO: -6.82462 LUMO: 1.86670 factor:1 | -1 (0.66352) | 1 | 1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.47336 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.69438) | 1 | 1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06737 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-0.28839) | 1 | 1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.73215 HOMO: -6.84094 LUMO: 1.27349 factor:1 | -1 (0.04683) | -1 | -1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58045 HOMO: -7.07768 LUMO: 1.27621 factor:1 | -1 (0.19853) | -1 | -1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.13409 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.35511) | -1 | -1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.21979 HOMO: -6.94162 LUMO: 1.64629 factor:1 | -1 (0.55919) | 1 | 1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23001 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.45103) | 1 | 1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91504 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.13606) | 1 | 1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60785 HOMO: -7.09129 LUMO: 1.73609 factor:1 | -1 (0.17113) | 1 | 1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50901 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-0.73003) | 1 | 1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.43694 HOMO: -6.93618 LUMO: 1.63540 factor:1 | -1 (1.34204) | 1 | 1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64148 HOMO: -6.98516 LUMO: 1.64629 factor:1 | -1 (0.13750) | 1 | 1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06745 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.28847) | 1 | 1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.52240 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.74342) | 1 | 1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.99615 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-1.21717) | 1 | 1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.96638 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.18740) | 1 | 1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.67364 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.89466) | 1 | 1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.03794 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-1.25896) | 1 | 1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.34053 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.56155) | -1 | -1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.76482 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.98584) | 1 | 1 |
| G: -6695.41329 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.23849 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.45951) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.63066 HOMO: -7.06135 LUMO: 0.75376 factor:1 | 1 (-1.85168) | 1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.26897 HOMO: -5.10213 LUMO: 0.77825 factor:1 | 1 (-1.48999) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76568 HOMO: -5.84228 LUMO: 0.50341 factor:1 | -1 (0.01331) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.55027 HOMO: -5.39874 LUMO: 0.68028 factor:1 | -1 (0.22871) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58080 HOMO: -5.16744 LUMO: 1.14832 factor:1 | -1 (0.19818) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.98884 HOMO: -5.80963 LUMO: 0.35647 factor:1 | -1 (0.79014) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79388 HOMO: -5.02322 LUMO: 1.07213 factor:1 | 1 (-1.01490) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89009 HOMO: -5.80963 LUMO: 0.56328 factor:1 | 1 (-0.11110) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.38101 HOMO: -5.45316 LUMO: 0.78369 factor:1 | 1 (-0.60202) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.28739 HOMO: -5.25452 LUMO: 0.82178 factor:1 | 1 (-1.50841) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.73369 HOMO: -5.21370 LUMO: 1.03947 factor:1 | 1 (-0.95471) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.37131 HOMO: -6.04365 LUMO: 0.31837 factor:1 | 1 (-1.59233) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.40278 HOMO: -5.86405 LUMO: 0.55511 factor:1 | 1 (-0.62379) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.78635 HOMO: -5.64908 LUMO: 0.71022 factor:1 | 1 (-1.00737) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.00843 HOMO: -5.94297 LUMO: 0.68301 factor:1 | 1 (-0.22945) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85730 HOMO: -6.01916 LUMO: 0.56328 factor:1 | 1 (-0.07831) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.74374 HOMO: -6.05181 LUMO: 0.35103 factor:1 | -1 (0.03524) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.49966 HOMO: -6.08447 LUMO: 0.48436 factor:1 | -1 (0.27932) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52156 HOMO: -5.86950 LUMO: 0.36735 factor:1 | -1 (0.25742) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69710 HOMO: -5.33615 LUMO: 0.65852 factor:1 | -1 (0.08188) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.56265 HOMO: -5.36064 LUMO: 0.86804 factor:1 | -1 (0.21633) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.08860 HOMO: -5.74160 LUMO: 0.64491 factor:1 | -1 (0.69038) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91175 HOMO: -5.23003 LUMO: 0.66124 factor:1 | 1 (-0.13276) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.04214 HOMO: -5.77698 LUMO: 0.84083 factor:1 | 1 (-0.26316) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70782 HOMO: -5.60555 LUMO: 0.84355 factor:1 | -1 (0.07116) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52477 HOMO: -7.11578 LUMO: -1.62452 factor:1 | -1 (0.25421) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.56113 HOMO: -7.23279 LUMO: -1.63813 factor:1 | -1 (0.21785) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.96860 HOMO: -6.68312 LUMO: -0.88709 factor:1 | -1 (0.81038) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.39513 HOMO: -6.99333 LUMO: -0.88709 factor:1 | 1 (-0.61615) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30302 HOMO: -7.40694 LUMO: 0.11973 factor:1 | 1 (-0.52404) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.71576 HOMO: -6.74026 LUMO: -0.72927 factor:1 | 1 (-0.93678) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.99762 HOMO: -6.67223 LUMO: -0.70750 factor:1 | 1 (-1.21863) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.71475 HOMO: -7.06952 LUMO: -1.40139 factor:1 | 1 (-1.93576) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.00222 HOMO: -7.21374 LUMO: -1.13199 factor:1 | 1 (-1.22323) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.56903 HOMO: -6.54706 LUMO: -1.34424 factor:1 | 1 (-1.79005) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14680 HOMO: -7.51851 LUMO: -1.05852 factor:1 | 1 (-0.36782) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.72518 HOMO: -7.07224 LUMO: -1.89391 factor:1 | 1 (-0.94619) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.71633 HOMO: -6.65863 LUMO: -0.46804 factor:1 | 1 (-0.93735) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50887 HOMO: -7.24367 LUMO: 0.29388 factor:1 | 1 (-0.72989) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79271 HOMO: -7.02326 LUMO: -0.87893 factor:1 | 1 (-1.01373) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.18244 HOMO: -6.88176 LUMO: 0.71566 factor:1 | 1 (-1.40345) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.10341 HOMO: -6.46543 LUMO: 1.01498 factor:1 | 1 (-1.32443) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.09871 HOMO: -6.30760 LUMO: 0.17687 factor:1 | 1 (-1.31973) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.03749 HOMO: -6.73210 LUMO: -1.06941 factor:1 | 1 (-0.25851) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06182 HOMO: -6.83550 LUMO: -0.75920 factor:1 | 1 (-0.28284) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.56015 HOMO: -6.94707 LUMO: 0.42178 factor:1 | -1 (0.21883) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.71044 HOMO: -6.77019 LUMO: -0.38096 factor:1 | -1 (0.06855) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06837 HOMO: -7.34163 LUMO: 0.35103 factor:1 | 1 (-0.28939) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.00930 HOMO: -6.87632 LUMO: -0.87349 factor:1 | 1 (-0.23032) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58905 HOMO: -7.06952 LUMO: -1.47214 factor:1 | -1 (0.18994) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62431 HOMO: -6.58788 LUMO: -0.37824 factor:1 | -1 (0.15467) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77846 HOMO: -6.92802 LUMO: -1.24900 factor:1 | -1 (0.00052) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.12867 HOMO: -7.01237 LUMO: -1.31975 factor:1 | 1 (-1.34968) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.09098 HOMO: -6.74842 LUMO: 0.45987 factor:1 | 1 (-1.31200) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.49044 HOMO: -6.53890 LUMO: 0.94424 factor:1 | 1 (-1.71146) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.65080 HOMO: -6.52257 LUMO: -0.66940 factor:1 | 1 (-1.87182) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.52835 HOMO: -6.56883 LUMO: -1.48302 factor:1 | 1 (-1.74937) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.36824 HOMO: -7.21646 LUMO: 0.13061 factor:1 | 1 (-1.58925) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.68802 HOMO: -6.62597 LUMO: -0.64763 factor:1 | 1 (-1.90904) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.67687 HOMO: -7.38789 LUMO: 0.31021 factor:1 | 1 (-1.89789) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.73821 HOMO: -6.74570 LUMO: -0.70750 factor:1 | 1 (-0.95923) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.48190 HOMO: -6.95251 LUMO: -1.25989 factor:1 | 1 (-1.70292) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.88447 HOMO: -7.13483 LUMO: -0.76736 factor:1 | 1 (-1.10549) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.04639 HOMO: -6.93618 LUMO: -1.24628 factor:1 | 1 (-0.26741) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05444 HOMO: -7.03686 LUMO: 0.26395 factor:1 | 1 (-0.27546) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58086 HOMO: -6.52257 LUMO: -0.84355 factor:1 | -1 (0.19813) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68521 HOMO: -6.83278 LUMO: -0.49525 factor:1 | -1 (0.09377) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.53095 HOMO: -7.18381 LUMO: -1.64629 factor:1 | -1 (0.24803) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.34662 HOMO: -6.74842 LUMO: -0.81090 factor:1 | -1 (0.43236) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17540 HOMO: -7.09401 LUMO: -0.92519 factor:1 | 1 (-0.39642) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.17830 HOMO: -7.20285 LUMO: -0.81634 factor:1 | 1 (-1.39932) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.32792 HOMO: -6.72665 LUMO: 0.77008 factor:1 | 1 (-0.54894) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.05574 HOMO: -6.80829 LUMO: 0.86532 factor:1 | 1 (-1.27676) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.31724 HOMO: -6.20964 LUMO: 0.99866 factor:1 | 1 (-1.53826) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.46084 HOMO: -6.52801 LUMO: 1.07757 factor:1 | 1 (-0.68186) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.31924 HOMO: -6.74298 LUMO: -0.67756 factor:1 | 1 (-0.54025) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.01220 HOMO: -7.43959 LUMO: 0.03265 factor:1 | 1 (-1.23322) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50452 HOMO: -6.46815 LUMO: -0.29933 factor:1 | 1 (-0.72554) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.66818 HOMO: -6.70489 LUMO: -0.97145 factor:1 | -1 (0.11080) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.72578 HOMO: -6.30216 LUMO: -1.39322 factor:1 | -1 (0.05320) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.63538 HOMO: -7.01782 LUMO: -1.07485 factor:1 | 1 (-0.85640) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.04173 HOMO: -6.93074 LUMO: 0.25851 factor:1 | 1 (-1.26274) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79759 HOMO: -7.07224 LUMO: 0.09524 factor:1 | 1 (-1.01860) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76706 HOMO: -6.62325 LUMO: -0.45443 factor:1 | -1 (0.01192) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59792 HOMO: -7.09945 LUMO: -1.20274 factor:1 | -1 (0.18106) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.70390 HOMO: -6.56067 LUMO: -1.39322 factor:1 | 1 (-0.92492) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.78368 HOMO: -6.75387 LUMO: -0.72654 factor:1 | 1 (-1.00470) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.42952 HOMO: -6.28583 LUMO: -2.35651 factor:1 | 1 (-0.65054) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.76266 HOMO: -6.55522 LUMO: -1.33608 factor:1 | -1 (1.01632) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.66984 HOMO: -7.19741 LUMO: -0.93607 factor:1 | -1 (0.10914) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.37815 HOMO: -6.39740 LUMO: -1.14832 factor:1 | 1 (-0.59917) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.51881 HOMO: -7.11850 LUMO: -0.97417 factor:1 | -1 (0.26017) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.91049 HOMO: -6.57699 LUMO: -1.14016 factor:1 | 1 (-1.13150) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.07384 HOMO: -6.57699 LUMO: -1.31975 factor:1 | 1 (-1.29485) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45810 HOMO: -6.69128 LUMO: -0.76736 factor:1 | -1 (0.32088) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61617 HOMO: -7.25728 LUMO: 0.29660 factor:1 | 1 (-0.83719) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.04017 HOMO: -6.37019 LUMO: -0.95240 factor:1 | -1 (0.73882) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.30123 HOMO: -6.48447 LUMO: -0.55511 factor:1 | -1 (0.47775) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.87318 HOMO: -6.37291 LUMO: -0.78641 factor:1 | 1 (-1.09420) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.45252 HOMO: -6.65863 LUMO: -0.69933 factor:1 | 1 (-0.67354) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.04880 HOMO: -6.44638 LUMO: -0.16055 factor:1 | 1 (-1.26982) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.59189 HOMO: -6.41917 LUMO: -0.20136 factor:1 | 1 (-0.81291) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.77973 HOMO: -7.33347 LUMO: 0.12789 factor:1 | 1 (-1.00075) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17442 HOMO: -6.70489 LUMO: -0.52518 factor:1 | 1 (-0.39544) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57982 HOMO: -7.25183 LUMO: 0.32109 factor:1 | -1 (0.19916) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68630 HOMO: -7.29265 LUMO: 0.28028 factor:1 | -1 (0.09268) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.45831 HOMO: -6.57155 LUMO: -0.51702 factor:1 | 1 (-0.67933) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.28711 HOMO: -7.08040 LUMO: 0.39729 factor:1 | -1 (0.49187) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58747 HOMO: -6.24501 LUMO: -0.44627 factor:1 | -1 (0.19151) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.86653 HOMO: -6.73754 LUMO: -0.45443 factor:1 | -1 (0.91245) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88976 HOMO: -6.24501 LUMO: 0.38096 factor:1 | 1 (-0.11078) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.37310 HOMO: -6.86815 LUMO: -0.91974 factor:1 | -1 (0.40589) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96312 HOMO: -7.40150 LUMO: 0.36191 factor:1 | 1 (-0.18414) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.02123 HOMO: -6.44094 LUMO: -0.64219 factor:1 | -1 (0.75776) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.71464 HOMO: -6.69944 LUMO: -0.80001 factor:1 | -1 (1.06435) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69629 HOMO: -6.61509 LUMO: -0.70750 factor:1 | -1 (0.08270) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.92206 HOMO: -7.52123 LUMO: 0.06803 factor:1 | 1 (-0.14308) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27024 HOMO: -7.34163 LUMO: 0.30477 factor:1 | -1 (0.50874) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.98675 HOMO: -6.68584 LUMO: -0.78641 factor:1 | -1 (0.79223) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69751 HOMO: -6.53890 LUMO: -0.50885 factor:1 | -1 (0.08147) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05039 HOMO: -6.75659 LUMO: -0.68845 factor:1 | 1 (-0.27141) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.62327 HOMO: -7.08857 LUMO: 0.43266 factor:1 | 1 (-0.84429) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88383 HOMO: -6.28583 LUMO: -0.46804 factor:1 | 1 (-0.10485) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.55737 HOMO: -6.50080 LUMO: -0.24762 factor:1 | -1 (0.22161) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.26983 HOMO: -6.45454 LUMO: -0.58504 factor:1 | -1 (0.50915) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59345 HOMO: -7.20558 LUMO: 0.20953 factor:1 | -1 (0.18553) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46572 HOMO: -6.35930 LUMO: -0.20681 factor:1 | -1 (0.31326) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70061 HOMO: -6.36202 LUMO: -0.14422 factor:1 | -1 (0.07837) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81909 HOMO: -6.20692 LUMO: 1.97827 factor:1 | 1 (-0.04011) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.02703 HOMO: -6.48719 LUMO: 1.74153 factor:1 | 1 (-1.24805) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.29177 HOMO: -6.84638 LUMO: 1.88575 factor:1 | 1 (-1.51279) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61236 HOMO: -5.90759 LUMO: 2.00820 factor:1 | 1 (-0.83338) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36473 HOMO: -6.56339 LUMO: 1.99732 factor:1 | 1 (-0.58575) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77212 HOMO: -6.20692 LUMO: 1.75241 factor:1 | -1 (0.00686) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.24160 HOMO: -6.16882 LUMO: 1.94017 factor:1 | 1 (-0.46262) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.66635 HOMO: -6.80829 LUMO: 1.78507 factor:1 | -1 (0.11263) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27451 HOMO: -6.58243 LUMO: 1.78235 factor:1 | -1 (0.50447) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05463 HOMO: -5.85045 LUMO: 1.82316 factor:1 | 1 (-0.27565) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58706 HOMO: -5.93752 LUMO: 1.56465 factor:1 | -1 (0.19192) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81041 HOMO: -6.59604 LUMO: -0.53334 factor:1 | 1 (-0.03143) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.75579 HOMO: -7.06135 LUMO: 0.29660 factor:1 | 1 (-0.97681) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.23822 HOMO: -6.50352 LUMO: 1.61908 factor:1 | 1 (-1.45924) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.67630 HOMO: -6.68040 LUMO: -0.60681 factor:1 | 1 (-0.89732) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.47872 HOMO: -6.93618 LUMO: -1.09662 factor:1 | 1 (-0.69974) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.69481 HOMO: -6.72121 LUMO: -1.14016 factor:1 | 1 (-0.91583) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27119 HOMO: -7.12394 LUMO: -1.24900 factor:1 | -1 (0.50779) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.04114 HOMO: -6.71305 LUMO: -0.71566 factor:1 | -1 (0.73784) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.31160 HOMO: -7.09401 LUMO: -0.86532 factor:1 | -1 (0.46738) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.42537 HOMO: -7.08584 LUMO: -0.92519 factor:1 | -1 (0.35361) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.24509 HOMO: -7.05591 LUMO: 0.11973 factor:1 | -1 (0.53389) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.26678 HOMO: -7.14843 LUMO: -1.58370 factor:1 | -1 (0.51220) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.22085 HOMO: -7.36884 LUMO: -1.97010 factor:1 | -1 (0.55813) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79440 HOMO: -6.81373 LUMO: -1.72248 factor:1 | 1 (-1.01542) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80168 HOMO: -6.87360 LUMO: -1.03947 factor:1 | 1 (-0.02269) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.37692 HOMO: -7.02870 LUMO: -0.87349 factor:1 | 1 (-1.59793) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.64773 HOMO: -7.16476 LUMO: -1.18097 factor:1 | 1 (-0.86875) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.39358 HOMO: -7.51851 LUMO: 0.07891 factor:1 | 1 (-0.61460) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.70537 HOMO: -7.04231 LUMO: -0.83539 factor:1 | 1 (-0.92638) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.38289 HOMO: -6.83278 LUMO: -0.60137 factor:1 | -1 (0.39609) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.43651 HOMO: -6.89809 LUMO: -1.19186 factor:1 | -1 (1.34247) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.10047 HOMO: -7.16476 LUMO: -0.79185 factor:1 | -1 (0.67852) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.40044 HOMO: -6.97156 LUMO: -1.25444 factor:1 | 1 (-0.62145) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.56842 HOMO: -6.84366 LUMO: -0.88437 factor:1 | -1 (0.21056) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.37214 HOMO: -6.91986 LUMO: -1.12655 factor:1 | -1 (0.40684) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.12261 HOMO: -6.49536 LUMO: -0.29660 factor:1 | 1 (-0.34363) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.18441 HOMO: -6.74842 LUMO: 0.42450 factor:1 | -1 (0.59457) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.38574 HOMO: -7.34435 LUMO: 0.32109 factor:1 | 1 (-0.60676) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.49870 HOMO: -7.16476 LUMO: 0.28572 factor:1 | -1 (0.28028) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.32858 HOMO: -6.74298 LUMO: -0.43538 factor:1 | -1 (0.45040) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11670 HOMO: -7.19469 LUMO: -1.61091 factor:1 | 1 (-0.33772) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.55808 HOMO: -7.35252 LUMO: -1.78235 factor:1 | -1 (0.22090) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.15156 HOMO: -7.25456 LUMO: -1.66806 factor:1 | 1 (-0.37258) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.25738 HOMO: -7.54844 LUMO: -1.07213 factor:1 | -1 (2.52160) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.97332 HOMO: -7.21918 LUMO: -1.55377 factor:1 | -1 (1.80567) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.61589 HOMO: -7.01782 LUMO: -1.60547 factor:1 | -1 (2.16309) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.92113 HOMO: -7.21646 LUMO: -1.53472 factor:1 | 1 (-0.14215) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45740 HOMO: -6.73754 LUMO: -1.37417 factor:1 | -1 (0.32158) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.13640 HOMO: -6.78924 LUMO: 0.66396 factor:1 | 1 (-0.35742) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.99145 HOMO: -6.82734 LUMO: 0.61226 factor:1 | 1 (-0.21247) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.61928 HOMO: -6.74026 LUMO: 0.65579 factor:1 | -1 (0.15970) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.36964 HOMO: -7.10489 LUMO: -1.30887 factor:1 | -1 (0.40934) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.02307 HOMO: -7.05047 LUMO: 0.42722 factor:1 | 1 (-0.24409) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.13224 HOMO: -6.61237 LUMO: 1.30887 factor:1 | 1 (-0.35326) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.04271 HOMO: -7.05863 LUMO: 0.59049 factor:1 | 1 (-0.26373) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.10205 HOMO: -6.26406 LUMO: 0.78641 factor:1 | -1 (1.67693) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76168 HOMO: -6.70489 LUMO: 0.67756 factor:1 | -1 (0.01731) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.64851 HOMO: -6.78652 LUMO: -0.94968 factor:1 | -1 (1.13047) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.11824 HOMO: -6.36202 LUMO: -0.94424 factor:1 | 1 (-1.33926) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23907 HOMO: -6.81645 LUMO: -1.09934 factor:1 | 1 (-0.46009) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.98208 HOMO: -7.07224 LUMO: 0.85988 factor:1 | 1 (-1.20310) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.07852 HOMO: -7.02326 LUMO: 1.10206 factor:1 | 1 (-0.29954) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.09800 HOMO: -6.71305 LUMO: 0.84627 factor:1 | 1 (-1.31902) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.22089 HOMO: -7.27360 LUMO: 0.88165 factor:1 | 1 (-0.44191) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.69873 HOMO: -6.84911 LUMO: 0.59865 factor:1 | 1 (-0.91974) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96549 HOMO: -6.75114 LUMO: -2.49801 factor:1 | 1 (-0.18651) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.20243 HOMO: -6.97156 LUMO: 0.53606 factor:1 | -1 (0.57655) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.80620 HOMO: -6.54434 LUMO: 0.73199 factor:1 | -1 (0.97278) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58086 HOMO: -6.21236 LUMO: 0.99866 factor:1 | -1 (0.19813) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.93403 HOMO: -6.34025 LUMO: 0.50341 factor:1 | 1 (-0.15505) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.57238 HOMO: -6.59876 LUMO: -0.69389 factor:1 | 1 (-0.79340) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.82689 HOMO: -6.54978 LUMO: -1.00682 factor:1 | 1 (-1.04791) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14043 HOMO: -6.82462 LUMO: -0.98777 factor:1 | 1 (-0.36145) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80535 HOMO: -6.85455 LUMO: -0.68573 factor:1 | 1 (-0.02637) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.70413 HOMO: -7.55388 LUMO: -0.03265 factor:1 | -1 (1.07485) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.90834 HOMO: -6.77019 LUMO: -0.71838 factor:1 | 1 (-0.12936) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.22364 HOMO: -6.84911 LUMO: -1.25444 factor:1 | 1 (-0.44466) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.76828 HOMO: -6.95251 LUMO: -1.03675 factor:1 | -1 (2.01070) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.34349 HOMO: -6.80829 LUMO: -0.77280 factor:1 | -1 (0.43549) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.94209 HOMO: -6.94162 LUMO: -0.94151 factor:1 | 1 (-0.16311) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.09998 HOMO: -6.89809 LUMO: -0.90886 factor:1 | -1 (0.67901) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.76236 HOMO: -6.85183 LUMO: -0.88981 factor:1 | -1 (1.01662) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.63512 HOMO: -6.51985 LUMO: -0.84627 factor:1 | -1 (0.14387) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69259 HOMO: -6.83278 LUMO: -1.08029 factor:1 | -1 (0.08640) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58951 HOMO: -6.91986 LUMO: 0.66396 factor:1 | -1 (0.18947) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.49040 HOMO: -6.94162 LUMO: 0.50885 factor:1 | -1 (0.28858) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.90218 HOMO: -6.94435 LUMO: 0.80546 factor:1 | -1 (0.87681) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85215 HOMO: -6.74298 LUMO: -0.81634 factor:1 | 1 (-0.07317) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.20697 HOMO: -7.04503 LUMO: 1.15921 factor:1 | -1 (0.57201) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.07647 HOMO: -6.76475 LUMO: 0.75920 factor:1 | -1 (0.70252) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62143 HOMO: -7.05047 LUMO: 0.68845 factor:1 | -1 (0.15755) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.74631 HOMO: -7.12666 LUMO: 0.60681 factor:1 | -1 (1.03267) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01597 HOMO: -6.90897 LUMO: -1.22723 factor:1 | 1 (-0.23698) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.95011 HOMO: -7.10761 LUMO: 0.58232 factor:1 | 1 (-0.17113) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76018 HOMO: -6.57427 LUMO: 0.71294 factor:1 | -1 (0.01880) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.89576 HOMO: -6.22597 LUMO: 0.99322 factor:1 | -1 (1.88322) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60935 HOMO: -6.83550 LUMO: -0.77825 factor:1 | -1 (0.16964) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96617 HOMO: -7.14843 LUMO: 0.44627 factor:1 | 1 (-0.18719) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.09541 HOMO: -7.08040 LUMO: 0.78913 factor:1 | -1 (1.68357) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.08568 HOMO: -6.81373 LUMO: -0.93879 factor:1 | 1 (-0.30670) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.67724 HOMO: -6.95251 LUMO: 0.22585 factor:1 | -1 (0.10174) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.58516 HOMO: -7.13483 LUMO: -1.25444 factor:1 | -1 (1.19382) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.33628 HOMO: -6.37835 LUMO: -1.54289 factor:1 | -1 (0.44270) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.51972 HOMO: -6.53617 LUMO: -1.43948 factor:1 | -1 (1.25926) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.53351 HOMO: -6.38379 LUMO: 0.16055 factor:1 | -1 (0.24547) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45198 HOMO: -6.53617 LUMO: 0.15783 factor:1 | -1 (0.32700) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.37565 HOMO: -6.79740 LUMO: -0.17960 factor:1 | -1 (0.40333) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.90829 HOMO: -6.26678 LUMO: -0.41361 factor:1 | 1 (-0.12931) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.67283 HOMO: -6.35658 LUMO: -0.24218 factor:1 | -1 (0.10615) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96062 HOMO: -6.48175 LUMO: -0.71566 factor:1 | 1 (-0.18164) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.75634 HOMO: -6.21508 LUMO: -0.40001 factor:1 | -1 (0.02264) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.98609 HOMO: -6.51985 LUMO: -0.32654 factor:1 | 1 (-0.20711) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.78306 HOMO: -6.45182 LUMO: -0.66396 factor:1 | 1 (-0.00408) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.74805 HOMO: -6.51441 LUMO: -0.65307 factor:1 | -1 (1.03093) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.53781 HOMO: -6.57971 LUMO: -0.92519 factor:1 | -1 (0.24117) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.55896 HOMO: -6.67223 LUMO: -0.58232 factor:1 | -1 (1.22002) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.21162 HOMO: -6.10351 LUMO: -0.45987 factor:1 | -1 (0.56736) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.28574 HOMO: -6.13889 LUMO: -0.50341 factor:1 | -1 (2.49324) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.93187 HOMO: -6.63141 LUMO: -0.28300 factor:1 | -1 (1.84711) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.64926 HOMO: -6.37563 LUMO: -0.22858 factor:1 | -1 (2.12973) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77901 HOMO: -6.37019 LUMO: 0.11429 factor:1 | 1 (-0.00003) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57408 HOMO: -6.23957 LUMO: 0.28844 factor:1 | -1 (0.20490) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.82932 HOMO: -6.41372 LUMO: -0.53879 factor:1 | 1 (-0.05034) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.92955 HOMO: -7.06680 LUMO: 0.32654 factor:1 | -1 (0.84943) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.78731 HOMO: -6.50896 LUMO: -0.73743 factor:1 | 1 (-0.00833) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69109 HOMO: -6.42189 LUMO: -0.28572 factor:1 | -1 (0.08789) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.56336 HOMO: -6.79740 LUMO: -0.25851 factor:1 | -1 (0.21562) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.97395 HOMO: -6.32393 LUMO: 0.17960 factor:1 | 1 (-0.19497) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89267 HOMO: -6.65046 LUMO: 0.03537 factor:1 | 1 (-0.11369) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.95294 HOMO: -6.60148 LUMO: 0.07619 factor:1 | 1 (-0.17396) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.19138 HOMO: -6.57971 LUMO: 0.11429 factor:1 | -1 (0.58760) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.25718 HOMO: -6.88448 LUMO: -1.21907 factor:1 | -1 (1.52180) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.36872 HOMO: -6.97700 LUMO: 0.36463 factor:1 | -1 (0.41027) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.50075 HOMO: -6.73210 LUMO: -0.84083 factor:1 | -1 (1.27823) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46605 HOMO: -6.21236 LUMO: -0.68845 factor:1 | -1 (0.31293) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.27861 HOMO: -6.35658 LUMO: -0.82995 factor:1 | 1 (-0.49963) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.33692 HOMO: -6.75114 LUMO: -0.94424 factor:1 | 1 (-0.55794) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62004 HOMO: -6.74026 LUMO: -1.46125 factor:1 | -1 (0.15894) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61992 HOMO: -7.06952 LUMO: 0.91974 factor:1 | 1 (-0.84094) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.92252 HOMO: -7.08857 LUMO: 0.74559 factor:1 | 1 (-0.14354) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.02664 HOMO: -6.74298 LUMO: 1.03131 factor:1 | -1 (0.75234) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.61884 HOMO: -6.74842 LUMO: -1.77962 factor:1 | -1 (0.16014) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.97738 HOMO: -6.82462 LUMO: -1.61908 factor:1 | 1 (-0.19840) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.94568 HOMO: -7.17020 LUMO: -1.02043 factor:1 | 1 (-0.16670) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.38009 HOMO: -6.26406 LUMO: -0.96328 factor:1 | -1 (0.39889) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.65612 HOMO: -6.50896 LUMO: -0.38640 factor:1 | -1 (0.12286) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.54224 HOMO: -7.27632 LUMO: -1.17553 factor:1 | -1 (0.23674) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.95695 HOMO: -6.54162 LUMO: -1.36873 factor:1 | -1 (0.82203) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80823 HOMO: -6.42733 LUMO: -1.15648 factor:1 | 1 (-0.02925) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.24216 HOMO: -6.73754 LUMO: -2.58780 factor:1 | -1 (0.53683) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.97998 HOMO: -7.20285 LUMO: 0.75103 factor:1 | 1 (-1.20100) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17336 HOMO: -6.98788 LUMO: 0.34831 factor:1 | 1 (-0.39437) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.98513 HOMO: -6.80013 LUMO: -1.11567 factor:1 | 1 (-1.20614) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01308 HOMO: -6.67767 LUMO: -0.82450 factor:1 | 1 (-0.23410) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23692 HOMO: -6.84911 LUMO: -0.21497 factor:1 | 1 (-0.45794) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.04978 HOMO: -6.23141 LUMO: 0.21769 factor:1 | 1 (-1.27080) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.55709 HOMO: -6.68312 LUMO: 0.16327 factor:1 | 1 (-0.77811) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91942 HOMO: -7.04503 LUMO: -1.04220 factor:1 | 1 (-0.14044) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.10855 HOMO: -6.67495 LUMO: -0.71294 factor:1 | -1 (0.67043) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.02729 HOMO: -6.70216 LUMO: -0.55239 factor:1 | 1 (-0.24830) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.94466 HOMO: -6.60420 LUMO: -0.71294 factor:1 | 1 (-1.16568) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.56419 HOMO: -7.40694 LUMO: 0.11973 factor:1 | 1 (-0.78521) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.97931 HOMO: -6.58788 LUMO: -0.29116 factor:1 | 1 (-0.20033) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.94088 HOMO: -6.63686 LUMO: -0.32654 factor:1 | 1 (-1.16190) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.57943 HOMO: -6.85183 LUMO: -0.95512 factor:1 | 1 (-0.80045) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.94750 HOMO: -6.82189 LUMO: -0.88165 factor:1 | 1 (-0.16852) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.60166 HOMO: -6.97428 LUMO: -1.03947 factor:1 | 1 (-0.82268) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.09284 HOMO: -6.51441 LUMO: -0.05714 factor:1 | 1 (-0.31386) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.95866 HOMO: -6.61509 LUMO: -0.77008 factor:1 | 1 (-0.17968) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.24833 HOMO: -7.36340 LUMO: 0.29116 factor:1 | -1 (0.53065) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87479 HOMO: -6.64230 LUMO: -0.79185 factor:1 | 1 (-0.09581) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.67055 HOMO: -6.56883 LUMO: -1.03403 factor:1 | -1 (1.10843) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.05802 HOMO: -6.69400 LUMO: -0.77825 factor:1 | -1 (0.72097) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.87593 HOMO: -6.37019 LUMO: -0.79185 factor:1 | -1 (1.90306) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01156 HOMO: -6.49808 LUMO: -0.94424 factor:1 | 1 (-0.23258) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.65708 HOMO: -6.91713 LUMO: -0.75376 factor:1 | -1 (1.12190) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.84233 HOMO: -7.13755 LUMO: 0.41361 factor:1 | 1 (-0.06335) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.79991 HOMO: -7.12122 LUMO: 0.39457 factor:1 | 1 (-0.02093) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91145 HOMO: -6.59332 LUMO: -0.57144 factor:1 | 1 (-0.13247) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.07205 HOMO: -6.62325 LUMO: -0.66940 factor:1 | 1 (-0.29307) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.12973 HOMO: -6.90897 LUMO: -0.08708 factor:1 | -1 (1.64925) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.81083 HOMO: -6.65591 LUMO: -0.81090 factor:1 | -1 (0.96815) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68695 HOMO: -6.65318 LUMO: -0.94696 factor:1 | -1 (0.09203) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.43514 HOMO: -6.96067 LUMO: -1.03675 factor:1 | -1 (0.34384) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68140 HOMO: -6.23141 LUMO: -0.66396 factor:1 | -1 (0.09758) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.29108 HOMO: -6.52529 LUMO: -0.78369 factor:1 | -1 (0.48790) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.90838 HOMO: -6.39468 LUMO: -0.40817 factor:1 | -1 (0.87060) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.66348 HOMO: -6.76203 LUMO: -0.20409 factor:1 | -1 (1.11550) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.84064 HOMO: -6.96611 LUMO: -0.90342 factor:1 | 1 (-0.06166) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80921 HOMO: -6.54706 LUMO: -0.87893 factor:1 | 1 (-0.03023) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.10993 HOMO: -7.24367 LUMO: -0.97689 factor:1 | 1 (-0.33094) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.86388 HOMO: -6.61781 LUMO: 1.43404 factor:1 | 1 (-0.08490) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.14634 HOMO: -6.17971 LUMO: 1.79867 factor:1 | -1 (0.63264) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45576 HOMO: -5.73344 LUMO: 2.13609 factor:1 | -1 (0.32322) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.52639 HOMO: -6.72121 LUMO: 2.06807 factor:1 | -1 (1.25259) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.61840 HOMO: -6.91169 LUMO: 2.02997 factor:1 | -1 (2.16058) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87890 HOMO: -7.06408 LUMO: 1.41499 factor:1 | 1 (-0.09992) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.86932 HOMO: -6.94162 LUMO: -0.90070 factor:1 | 1 (-0.09034) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64967 HOMO: -7.09401 LUMO: 0.35103 factor:1 | -1 (0.12931) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59413 HOMO: -6.78652 LUMO: 0.91974 factor:1 | -1 (0.18485) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60826 HOMO: -6.32937 LUMO: -1.89119 factor:1 | -1 (0.17072) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.61672 HOMO: -7.12666 LUMO: -1.06397 factor:1 | -1 (0.16226) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.78384 HOMO: -6.38107 LUMO: -1.43132 factor:1 | 1 (-1.00486) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.33698 HOMO: -7.09129 LUMO: 0.08980 factor:1 | 1 (-0.55800) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62967 HOMO: -6.31304 LUMO: -0.57960 factor:1 | -1 (0.14931) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20190 HOMO: -6.94435 LUMO: -0.74287 factor:1 | 1 (-0.42292) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36838 HOMO: -6.35658 LUMO: -1.53472 factor:1 | 1 (-0.58940) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.57002 HOMO: -6.39740 LUMO: -1.48846 factor:1 | 1 (-0.79103) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.86293 HOMO: -7.05319 LUMO: -0.33198 factor:1 | 1 (-0.08395) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70861 HOMO: -6.68040 LUMO: -0.09252 factor:1 | -1 (0.07037) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30277 HOMO: -6.35930 LUMO: -0.43266 factor:1 | 1 (-0.52379) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50645 HOMO: -6.59604 LUMO: -1.45853 factor:1 | 1 (-0.72747) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45898 HOMO: -6.46270 LUMO: -1.49391 factor:1 | -1 (0.32001) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46330 HOMO: -7.05863 LUMO: -1.04764 factor:1 | -1 (0.31568) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.35614 HOMO: -7.14027 LUMO: -0.81634 factor:1 | 1 (-0.57715) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.72251 HOMO: -6.80285 LUMO: -0.74287 factor:1 | 1 (-0.94353) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52050 HOMO: -6.53890 LUMO: -1.13471 factor:1 | -1 (0.25848) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68597 HOMO: -6.49808 LUMO: -1.35513 factor:1 | -1 (0.09301) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11665 HOMO: -6.75931 LUMO: -1.49663 factor:1 | 1 (-0.33767) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.71686 HOMO: -6.84638 LUMO: -0.77552 factor:1 | -1 (0.06212) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70184 HOMO: -6.65863 LUMO: -1.34696 factor:1 | -1 (0.07714) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.84173 HOMO: -6.25590 LUMO: -2.36467 factor:1 | 1 (-0.06275) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.77983 HOMO: -7.24911 LUMO: 0.33470 factor:1 | -1 (0.99915) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.47857 HOMO: -6.65863 LUMO: -0.75648 factor:1 | -1 (0.30041) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62608 HOMO: -6.31576 LUMO: -0.83267 factor:1 | -1 (0.15290) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.39519 HOMO: -6.64774 LUMO: -0.66124 factor:1 | -1 (0.38379) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77719 HOMO: -6.75387 LUMO: -1.00138 factor:1 | -1 (0.00180) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.75977 HOMO: -6.52529 LUMO: -0.68301 factor:1 | -1 (0.01921) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.40375 HOMO: -6.59332 LUMO: -0.68028 factor:1 | -1 (2.37523) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89444 HOMO: -5.98650 LUMO: 0.31565 factor:1 | 1 (-0.11546) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76758 HOMO: -6.59876 LUMO: 0.22585 factor:1 | -1 (0.01140) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.66015 HOMO: -6.72121 LUMO: 0.10340 factor:1 | -1 (0.11883) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45710 HOMO: -6.09807 LUMO: 0.20136 factor:1 | -1 (0.32188) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.61768 HOMO: -6.31576 LUMO: 0.06259 factor:1 | -1 (1.16130) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.86847 HOMO: -6.35658 LUMO: -0.58232 factor:1 | 1 (-1.08949) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91063 HOMO: -6.34842 LUMO: -0.55783 factor:1 | 1 (-0.13165) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.12857 HOMO: -6.47359 LUMO: -0.57144 factor:1 | 1 (-0.34958) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46262 HOMO: -6.42189 LUMO: -0.09796 factor:1 | -1 (0.31636) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77700 HOMO: -6.35658 LUMO: -0.31293 factor:1 | -1 (0.00199) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.92074 HOMO: -7.35524 LUMO: 0.10340 factor:1 | 1 (-1.14176) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.90108 HOMO: -7.10217 LUMO: 0.36463 factor:1 | 1 (-0.12210) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.85448 HOMO: -6.43549 LUMO: -0.56872 factor:1 | 1 (-1.07550) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17564 HOMO: -6.50080 LUMO: -0.71294 factor:1 | 1 (-0.39666) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50864 HOMO: -6.59060 LUMO: -0.57960 factor:1 | -1 (0.27035) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.28571 HOMO: -6.78924 LUMO: -0.31565 factor:1 | 1 (-0.50673) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80864 HOMO: -6.35658 LUMO: 0.07891 factor:1 | 1 (-0.02966) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62970 HOMO: -6.74026 LUMO: -0.87621 factor:1 | -1 (0.14928) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.36270 HOMO: -6.54434 LUMO: 0.81906 factor:1 | -1 (0.41628) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.38619 HOMO: -6.66135 LUMO: 1.40955 factor:1 | -1 (0.39280) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89670 HOMO: -6.73754 LUMO: -2.54971 factor:1 | 1 (-0.11772) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.36447 HOMO: -6.65318 LUMO: 0.69389 factor:1 | -1 (0.41451) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.15551 HOMO: -6.73482 LUMO: 0.62858 factor:1 | 1 (-0.37652) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.43410 HOMO: -6.83550 LUMO: 0.68573 factor:1 | -1 (0.34488) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.75460 HOMO: -6.83278 LUMO: 0.45987 factor:1 | -1 (0.02438) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.09850 HOMO: -6.78380 LUMO: 0.68301 factor:1 | 1 (-0.31952) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.34879 HOMO: -6.90625 LUMO: 1.36601 factor:1 | 1 (-0.56981) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52140 HOMO: -6.82734 LUMO: 1.48302 factor:1 | -1 (0.25758) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.36531 HOMO: -6.44094 LUMO: -0.94424 factor:1 | -1 (0.41367) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.42842 HOMO: -6.91441 LUMO: 0.28844 factor:1 | -1 (0.35056) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.52971 HOMO: -6.49808 LUMO: -0.51157 factor:1 | -1 (1.24927) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36887 HOMO: -7.09673 LUMO: -0.06259 factor:1 | 1 (-0.58989) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64121 HOMO: -6.77019 LUMO: 0.92247 factor:1 | -1 (0.13777) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20963 HOMO: -6.75931 LUMO: 1.13744 factor:1 | 1 (-0.43065) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27998 HOMO: -6.15794 LUMO: 1.12383 factor:1 | -1 (0.49900) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91847 HOMO: -6.59604 LUMO: 1.19458 factor:1 | 1 (-0.13949) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.77797 HOMO: -7.09401 LUMO: 0.60137 factor:1 | 1 (-0.99898) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.40737 HOMO: -6.34025 LUMO: 0.48164 factor:1 | 1 (-1.62838) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.15749 HOMO: -6.72665 LUMO: -2.47624 factor:1 | 1 (-0.37851) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.62558 HOMO: -6.48175 LUMO: 0.58232 factor:1 | 1 (-0.84660) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.41448 HOMO: -6.94162 LUMO: 0.28300 factor:1 | 1 (-0.63549) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.48097 HOMO: -6.65591 LUMO: 0.57144 factor:1 | 1 (-1.70199) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.84379 HOMO: -6.58788 LUMO: -1.03947 factor:1 | 1 (-1.06481) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.48689 HOMO: -7.18108 LUMO: 0.37824 factor:1 | 1 (-0.70790) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.99975 HOMO: -6.63958 LUMO: -1.52112 factor:1 | 1 (-0.22077) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46333 HOMO: -6.12528 LUMO: -0.53606 factor:1 | -1 (0.31565) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.91280 HOMO: -6.22324 LUMO: -0.87893 factor:1 | 1 (-1.13382) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11510 HOMO: -6.62053 LUMO: -0.91974 factor:1 | 1 (-0.33612) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.63297 HOMO: -6.84366 LUMO: -0.83811 factor:1 | 1 (-1.85399) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.93868 HOMO: -7.26000 LUMO: 0.25851 factor:1 | 1 (-1.15969) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.52000 HOMO: -6.49536 LUMO: -0.63403 factor:1 | 1 (-0.74102) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.72120 HOMO: -6.45726 LUMO: -0.77825 factor:1 | 1 (-0.94222) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.18657 HOMO: -6.74570 LUMO: -0.75103 factor:1 | 1 (-1.40759) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.55840 HOMO: -7.20285 LUMO: 0.10612 factor:1 | 1 (-0.77942) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.79132 HOMO: -6.45182 LUMO: -0.56600 factor:1 | 1 (-2.01234) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.84552 HOMO: -6.83278 LUMO: -0.71838 factor:1 | 1 (-2.06654) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.38163 HOMO: -7.01510 LUMO: -1.09662 factor:1 | 1 (-0.60265) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.66313 HOMO: -6.48719 LUMO: 0.16871 factor:1 | 1 (-0.88415) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.94981 HOMO: -7.30898 LUMO: 0.26667 factor:1 | 1 (-1.17082) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.21796 HOMO: -6.68856 LUMO: -0.78641 factor:1 | 1 (-0.43897) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.03471 HOMO: -6.56883 LUMO: -1.00682 factor:1 | 1 (-1.25572) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36177 HOMO: -6.41100 LUMO: -0.48980 factor:1 | 1 (-0.58279) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.97749 HOMO: -6.52257 LUMO: -0.59865 factor:1 | 1 (-0.19851) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.08554 HOMO: -6.63686 LUMO: -0.56055 factor:1 | 1 (-1.30655) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.09860 HOMO: -6.79740 LUMO: -0.75376 factor:1 | 1 (-1.31962) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.44950 HOMO: -5.89127 LUMO: 0.22313 factor:1 | 1 (-0.67052) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01771 HOMO: -6.34842 LUMO: 0.11429 factor:1 | 1 (-0.23873) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.48778 HOMO: -6.13617 LUMO: 1.94834 factor:1 | 1 (-1.70879) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.41771 HOMO: -6.50080 LUMO: 1.74153 factor:1 | 1 (-0.63873) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.12744 HOMO: -6.33481 LUMO: 1.68438 factor:1 | 1 (-1.34846) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.29902 HOMO: -6.53073 LUMO: 1.95106 factor:1 | 1 (-0.52004) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.32243 HOMO: -6.46270 LUMO: 1.89935 factor:1 | -1 (0.45655) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36653 HOMO: -5.87222 LUMO: 1.91568 factor:1 | 1 (-0.58755) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.23562 HOMO: -6.07630 LUMO: 1.81500 factor:1 | -1 (0.54336) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30226 HOMO: -6.20964 LUMO: 1.81500 factor:1 | 1 (-0.52327) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68350 HOMO: -6.15522 LUMO: 1.90752 factor:1 | -1 (0.09548) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.73081 HOMO: -6.11984 LUMO: 1.95378 factor:1 | 1 (-0.95183) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64360 HOMO: -6.58516 LUMO: 2.04358 factor:1 | -1 (0.13538) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.55361 HOMO: -7.37156 LUMO: 0.24490 factor:1 | 1 (-0.77463) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.29576 HOMO: -6.36474 LUMO: -0.90070 factor:1 | -1 (0.48322) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57313 HOMO: -6.43549 LUMO: -0.40817 factor:1 | -1 (0.20585) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20402 HOMO: -7.32258 LUMO: 0.29388 factor:1 | 1 (-0.42504) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27168 HOMO: -6.41372 LUMO: -0.20409 factor:1 | -1 (0.50730) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.41332 HOMO: -7.18381 LUMO: 0.42722 factor:1 | -1 (0.36567) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.96192 HOMO: -6.53890 LUMO: -0.54151 factor:1 | 1 (-1.18293) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61946 HOMO: -6.61509 LUMO: 0.08708 factor:1 | 1 (-0.84048) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50501 HOMO: -6.78108 LUMO: 2.03541 factor:1 | 1 (-0.72603) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.71266 HOMO: -6.50896 LUMO: 1.53472 factor:1 | 1 (-0.93368) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20000 HOMO: -6.65591 LUMO: 1.80411 factor:1 | 1 (-0.42101) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.15173 HOMO: -6.64502 LUMO: 1.52112 factor:1 | -1 (0.62725) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.38362 HOMO: -6.72938 LUMO: 1.48030 factor:1 | 1 (-0.60464) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.41356 HOMO: -6.16882 LUMO: 1.96466 factor:1 | -1 (0.36542) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17902 HOMO: -6.22597 LUMO: 1.43132 factor:1 | 1 (-0.40003) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.55212 HOMO: -6.57699 LUMO: 2.05718 factor:1 | -1 (0.22686) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64679 HOMO: -6.52529 LUMO: 1.89663 factor:1 | -1 (0.13219) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.97625 HOMO: -6.30760 LUMO: 1.88031 factor:1 | -1 (0.80274) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.78108 HOMO: -6.14977 LUMO: 1.92657 factor:1 | 1 (-0.00210) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.83139 HOMO: -6.20964 LUMO: 1.83949 factor:1 | 1 (-0.05241) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.18915 HOMO: -6.31848 LUMO: 1.91296 factor:1 | -1 (0.58983) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68897 HOMO: -5.80691 LUMO: 2.19868 factor:1 | -1 (0.09002) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.48445 HOMO: -6.00827 LUMO: 2.15514 factor:1 | -1 (0.29454) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.82630 HOMO: -6.51713 LUMO: 2.08711 factor:1 | 1 (-0.04732) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85049 HOMO: -6.32937 LUMO: 2.11705 factor:1 | 1 (-0.07151) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60619 HOMO: -6.26678 LUMO: 1.95922 factor:1 | -1 (0.17279) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.96493 HOMO: -6.43005 LUMO: 2.56603 factor:1 | -1 (0.81406) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64513 HOMO: -6.41644 LUMO: 2.68304 factor:1 | -1 (0.13385) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91517 HOMO: -5.97834 LUMO: 2.02997 factor:1 | 1 (-0.13619) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77659 HOMO: -6.14161 LUMO: 1.77690 factor:1 | -1 (0.00239) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.22588 HOMO: -6.21508 LUMO: 1.80411 factor:1 | -1 (0.55310) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76018 HOMO: -6.46270 LUMO: 2.34562 factor:1 | -1 (0.01880) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69691 HOMO: -6.39195 LUMO: -0.75920 factor:1 | -1 (0.08207) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50779 HOMO: -7.08584 LUMO: -1.14016 factor:1 | -1 (0.27119) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.78617 HOMO: -6.70216 LUMO: -0.65035 factor:1 | 1 (-0.00718) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85038 HOMO: -6.79468 LUMO: -0.83811 factor:1 | 1 (-0.07140) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.10897 HOMO: -6.99877 LUMO: -0.79729 factor:1 | 1 (-1.32998) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23409 HOMO: -7.08040 LUMO: -0.85444 factor:1 | 1 (-0.45511) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.62047 HOMO: -7.39333 LUMO: 0.12789 factor:1 | 1 (-0.84148) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.74325 HOMO: -7.05047 LUMO: 0.13878 factor:1 | -1 (0.03573) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.66594 HOMO: -6.90897 LUMO: -0.77552 factor:1 | 1 (-0.88696) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57038 HOMO: -7.25456 LUMO: 0.05170 factor:1 | -1 (0.20860) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.90790 HOMO: -6.84638 LUMO: -0.84355 factor:1 | 1 (-1.12892) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01553 HOMO: -6.78108 LUMO: -0.81634 factor:1 | 1 (-0.23655) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.80085 HOMO: -6.74570 LUMO: -0.77280 factor:1 | 1 (-1.02187) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80086 HOMO: -7.28177 LUMO: -1.68438 factor:1 | 1 (-0.02188) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50333 HOMO: -7.22190 LUMO: -1.63540 factor:1 | -1 (0.27565) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.71781 HOMO: -7.15932 LUMO: -1.57554 factor:1 | -1 (0.06117) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.78820 HOMO: -6.57971 LUMO: -0.93063 factor:1 | 1 (-1.00922) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.29681 HOMO: -6.88176 LUMO: 0.58232 factor:1 | 1 (-0.51783) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50899 HOMO: -6.85727 LUMO: 0.51430 factor:1 | -1 (0.26999) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.03004 HOMO: -6.83550 LUMO: 0.87893 factor:1 | -1 (0.74894) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59835 HOMO: -7.06680 LUMO: 0.87621 factor:1 | -1 (0.18063) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.52210 HOMO: -6.52257 LUMO: 0.81362 factor:1 | 1 (-0.74312) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.37761 HOMO: -6.95523 LUMO: 1.17009 factor:1 | -1 (0.40137) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.96747 HOMO: -7.21374 LUMO: 0.97145 factor:1 | 1 (-1.18848) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.56051 HOMO: -6.81373 LUMO: -1.54561 factor:1 | 1 (-1.78153) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.41821 HOMO: -6.86543 LUMO: -1.52656 factor:1 | -1 (0.36077) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.71622 HOMO: -6.90081 LUMO: -0.78097 factor:1 | 1 (-0.93724) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.48064 HOMO: -6.64502 LUMO: -0.82723 factor:1 | -1 (1.29834) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.72281 HOMO: -6.65591 LUMO: -0.82178 factor:1 | 1 (-0.94383) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.93552 HOMO: -6.79468 LUMO: -1.46397 factor:1 | 1 (-1.15654) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64282 HOMO: -7.25728 LUMO: 0.73743 factor:1 | -1 (0.13617) | 1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60178 HOMO: -7.00149 LUMO: 1.30070 factor:1 | -1 (0.17720) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62126 HOMO: -7.07768 LUMO: 0.78097 factor:1 | -1 (0.15772) | 1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.51776 HOMO: -6.86271 LUMO: 0.86260 factor:1 | 1 (-1.73878) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61864 HOMO: -6.94707 LUMO: 0.39729 factor:1 | 1 (-0.83966) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.21066 HOMO: -6.79740 LUMO: 0.67484 factor:1 | 1 (-0.43168) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.67475 HOMO: -6.91986 LUMO: -1.14288 factor:1 | 1 (-0.89577) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.24073 HOMO: -6.31576 LUMO: 1.01771 factor:1 | 1 (-0.46175) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.85606 HOMO: -6.81645 LUMO: 0.81362 factor:1 | 1 (-1.07708) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.44547 HOMO: -6.92258 LUMO: -0.99594 factor:1 | 1 (-0.66649) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.64594 HOMO: -6.81373 LUMO: 0.61770 factor:1 | 1 (-0.86695) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.26122 HOMO: -7.18653 LUMO: 1.19186 factor:1 | 1 (-0.48224) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.43488 HOMO: -7.00693 LUMO: 0.45715 factor:1 | 1 (-0.65590) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45326 HOMO: -7.11306 LUMO: 0.53334 factor:1 | -1 (0.32572) | 1 | 1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27641 HOMO: -6.63414 LUMO: -1.64357 factor:1 | -1 (0.50257) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70116 HOMO: -6.22052 LUMO: -0.74015 factor:1 | -1 (0.07782) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59963 HOMO: -6.81101 LUMO: -0.50069 factor:1 | -1 (0.17935) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59068 HOMO: -6.71849 LUMO: -0.51974 factor:1 | -1 (0.18830) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.92835 HOMO: -6.72121 LUMO: -1.77690 factor:1 | -1 (0.85063) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.65019 HOMO: -6.94162 LUMO: -1.78779 factor:1 | -1 (0.12879) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89858 HOMO: -6.91169 LUMO: 0.88981 factor:1 | 1 (-0.11959) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.44415 HOMO: -6.97428 LUMO: 0.70750 factor:1 | -1 (0.33484) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.33788 HOMO: -6.74842 LUMO: 1.15921 factor:1 | 1 (-0.55889) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.51021 HOMO: -7.25183 LUMO: -0.99594 factor:1 | -1 (0.26877) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.22642 HOMO: -6.43821 LUMO: -1.00410 factor:1 | 1 (-0.44744) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.72404 HOMO: -6.52257 LUMO: -0.68573 factor:1 | -1 (0.05494) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50015 HOMO: -6.60148 LUMO: -0.52518 factor:1 | -1 (0.27884) | -1 | -1 |
| G: -6695.41329 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.26107 HOMO: -6.07086 LUMO: -1.39594 factor:1 | -1 (0.51791) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.63887 HOMO: -6.78108 LUMO: -1.54833 factor:1 | 1 (-0.98122) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.02017 HOMO: -6.73482 LUMO: -1.01498 factor:1 | -1 (0.63748) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.96118 HOMO: -6.85183 LUMO: 1.06669 factor:1 | -1 (0.69648) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.84865 HOMO: -6.98516 LUMO: 1.43948 factor:1 | 1 (-0.19100) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.03949 HOMO: -6.94162 LUMO: 0.79185 factor:1 | 1 (-0.38183) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60491 HOMO: -6.67495 LUMO: -1.06669 factor:1 | 1 (-0.94726) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.94545 HOMO: -6.88720 LUMO: -1.00682 factor:1 | -1 (0.71220) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.22447 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-0.56681) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.35449 HOMO: -6.51713 LUMO: -0.89798 factor:1 | -1 (0.30316) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.47621 HOMO: -6.63141 LUMO: -0.91430 factor:1 | -1 (0.18145) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.99465 HOMO: -6.63414 LUMO: 0.04354 factor:1 | -1 (0.66301) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.57031 HOMO: -6.65046 LUMO: -0.73743 factor:1 | -1 (0.08735) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.71790 HOMO: -6.73754 LUMO: -0.71838 factor:1 | 1 (-0.06025) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.33816 HOMO: -6.65863 LUMO: -0.60137 factor:1 | 1 (-0.68050) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.89367 HOMO: -6.61509 LUMO: -0.47892 factor:1 | -1 (0.76399) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.38072 HOMO: -6.82189 LUMO: -0.64763 factor:1 | -1 (0.27693) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.69654 HOMO: -6.56883 LUMO: -0.51974 factor:1 | 1 (-0.03889) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.62337 HOMO: -6.97428 LUMO: -0.95512 factor:1 | -1 (0.03429) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.14289 HOMO: -6.70489 LUMO: -0.04082 factor:1 | 1 (-0.48523) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.51496 HOMO: -6.74026 LUMO: 0.02177 factor:1 | -1 (0.14270) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.77865 HOMO: -6.50080 LUMO: -0.89525 factor:1 | -1 (0.87901) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.98790 HOMO: -6.46815 LUMO: -0.61226 factor:1 | -1 (0.66975) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.61189 HOMO: -6.57971 LUMO: -0.64219 factor:1 | -1 (0.04577) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.86825 HOMO: -7.17836 LUMO: 0.37280 factor:1 | -1 (0.78940) | 1 | 1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.98287 HOMO: -6.67223 LUMO: 0.12245 factor:1 | -1 (0.67479) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.49322 HOMO: -6.55250 LUMO: 0.22858 factor:1 | -1 (0.16444) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.48845 HOMO: -6.97156 LUMO: -1.12927 factor:1 | -1 (0.16920) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.41879 HOMO: -6.78924 LUMO: -0.84900 factor:1 | -1 (0.23886) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.49959 HOMO: -6.65046 LUMO: -0.65307 factor:1 | -1 (1.15806) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.58626 HOMO: -7.41782 LUMO: 0.08980 factor:1 | -1 (1.07139) | 1 | 1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.73620 HOMO: -6.56339 LUMO: -0.68573 factor:1 | -1 (0.92146) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.77799 HOMO: -6.31032 LUMO: -0.31837 factor:1 | -1 (0.87966) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.43230 HOMO: -6.72938 LUMO: -0.45987 factor:1 | -1 (1.22536) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.84327 HOMO: -6.59876 LUMO: -1.03131 factor:1 | -1 (0.81438) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.37588 HOMO: -7.29265 LUMO: 0.29660 factor:1 | -1 (0.28177) | 1 | 1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.43419 HOMO: -6.42189 LUMO: -0.51157 factor:1 | -1 (0.22346) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.51915 HOMO: -6.27767 LUMO: -0.52790 factor:1 | -1 (0.13851) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.23035 HOMO: -6.41644 LUMO: -0.44627 factor:1 | -1 (0.42730) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.81380 HOMO: -6.23413 LUMO: -0.52790 factor:1 | -1 (0.84385) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.45841 HOMO: -6.63414 LUMO: -0.44082 factor:1 | -1 (0.19924) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.69975 HOMO: -7.03142 LUMO: 0.47076 factor:1 | 1 (-0.04210) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.45477 HOMO: -6.62053 LUMO: -0.14422 factor:1 | -1 (0.20289) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.60867 HOMO: -6.22324 LUMO: 1.96194 factor:1 | -1 (0.04898) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.27404 HOMO: -6.17971 LUMO: 1.71704 factor:1 | -1 (1.38362) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.54278 HOMO: -6.70761 LUMO: 1.68711 factor:1 | -1 (1.11488) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.69641 HOMO: -6.52801 LUMO: 1.56193 factor:1 | -1 (0.96124) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.84360 HOMO: -6.55794 LUMO: 1.52384 factor:1 | -1 (0.81406) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.70558 HOMO: -6.47359 LUMO: 1.82316 factor:1 | -1 (0.95207) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.40652 HOMO: -6.65863 LUMO: 1.83133 factor:1 | -1 (0.25113) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.87470 HOMO: -6.46270 LUMO: 1.90208 factor:1 | -1 (0.78295) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.00730 HOMO: -6.41917 LUMO: 2.03269 factor:1 | -1 (0.65035) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.38837 HOMO: -6.48992 LUMO: 1.87486 factor:1 | -1 (0.26928) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.34170 HOMO: -6.51985 LUMO: 1.69527 factor:1 | -1 (0.31595) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.42769 HOMO: -6.36202 LUMO: 2.05718 factor:1 | -1 (0.22996) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.60675 HOMO: -5.96474 LUMO: 1.88575 factor:1 | -1 (1.05090) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.81437 HOMO: -6.56339 LUMO: 2.04630 factor:1 | -1 (0.84328) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.77655 HOMO: -6.43277 LUMO: 1.98371 factor:1 | -1 (0.88110) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.05734 HOMO: -6.53345 LUMO: 2.06262 factor:1 | 1 (-0.39968) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.11902 HOMO: -5.81779 LUMO: 2.11432 factor:1 | 1 (-0.46137) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57136 HOMO: -5.91848 LUMO: 1.86942 factor:1 | 1 (-0.91370) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.43413 HOMO: -6.48447 LUMO: 1.70343 factor:1 | 1 (-0.77648) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70157 HOMO: -6.29671 LUMO: -0.89525 factor:1 | 1 (-1.04391) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.90530 HOMO: -6.63414 LUMO: -0.76192 factor:1 | 1 (-1.24764) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61590 HOMO: -6.56883 LUMO: -0.86260 factor:1 | 1 (-1.95824) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.32256 HOMO: -6.93074 LUMO: -0.27483 factor:1 | 1 (-1.66490) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.32286 HOMO: -6.85999 LUMO: -0.01905 factor:1 | 1 (-0.66521) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.32844 HOMO: -6.26406 LUMO: 0.21769 factor:1 | 1 (-0.67079) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14242 HOMO: -6.62325 LUMO: 0.31293 factor:1 | 1 (-1.48476) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.99322 HOMO: -6.59604 LUMO: 0.19592 factor:1 | 1 (-1.33556) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.22207 HOMO: -6.43277 LUMO: -0.27756 factor:1 | 1 (-0.56442) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.33846 HOMO: -6.54978 LUMO: -0.46531 factor:1 | 1 (-0.68080) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.19110 HOMO: -6.65046 LUMO: -0.15783 factor:1 | 1 (-1.53344) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17722 HOMO: -7.28721 LUMO: 0.23946 factor:1 | 1 (-1.51957) | 1 | 1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.02557 HOMO: -6.71849 LUMO: -0.56600 factor:1 | 1 (-1.36792) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.26425 HOMO: -6.85183 LUMO: -0.84355 factor:1 | 1 (-0.60660) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.19676 HOMO: -6.53345 LUMO: -0.84627 factor:1 | 1 (-1.53910) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.94447 HOMO: -6.60148 LUMO: -0.63130 factor:1 | 1 (-2.28682) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.17552 HOMO: -6.36202 LUMO: -0.60137 factor:1 | 1 (-2.51787) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.06907 HOMO: -6.28855 LUMO: -0.52790 factor:1 | 1 (-2.41142) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.90021 HOMO: -7.07224 LUMO: 0.41906 factor:1 | 1 (-1.24255) | 1 | 1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01561 HOMO: -6.36202 LUMO: -0.24218 factor:1 | 1 (-1.35796) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.39316 HOMO: -6.43549 LUMO: 0.14150 factor:1 | 1 (-2.73551) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.05207 HOMO: -6.76747 LUMO: -0.40545 factor:1 | 1 (-2.39441) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.34079 HOMO: -6.15249 LUMO: -0.51157 factor:1 | 1 (-1.68313) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.32166 HOMO: -6.33753 LUMO: -0.02993 factor:1 | 1 (-1.66400) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.29031 HOMO: -6.49808 LUMO: -0.83811 factor:1 | 1 (-1.63266) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.64528 HOMO: -6.64502 LUMO: -0.46259 factor:1 | 1 (-1.98763) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.64387 HOMO: -6.34570 LUMO: 0.22041 factor:1 | 1 (-1.98621) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.63356 HOMO: -6.63414 LUMO: -0.13606 factor:1 | 1 (-1.97590) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.56169 HOMO: -6.59604 LUMO: -0.79729 factor:1 | 1 (-1.90404) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.75075 HOMO: -7.09401 LUMO: 0.31837 factor:1 | 1 (-2.09310) | 1 | 1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.72543 HOMO: -6.48719 LUMO: -0.31021 factor:1 | 1 (-1.06777) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.08680 HOMO: -7.11306 LUMO: 0.39729 factor:1 | 1 (-1.42914) | 1 | 1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.07806 HOMO: -6.95251 LUMO: 0.41089 factor:1 | 1 (-1.42041) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61802 HOMO: -6.61509 LUMO: -0.41906 factor:1 | 1 (-1.96036) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.39189 HOMO: -6.25318 LUMO: -0.47348 factor:1 | 1 (-1.73424) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.46705 HOMO: -6.77019 LUMO: -0.10340 factor:1 | 1 (-1.80939) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50338 HOMO: -6.54706 LUMO: -0.46259 factor:1 | 1 (-1.84572) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.37259 HOMO: -6.34297 LUMO: -0.50341 factor:1 | -1 (0.28507) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.34846 HOMO: -6.20692 LUMO: -0.51974 factor:1 | 1 (-1.69081) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.27950 HOMO: -7.03686 LUMO: 0.46804 factor:1 | 1 (-2.62184) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.08262 HOMO: -6.47087 LUMO: 0.22585 factor:1 | 1 (-2.42497) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30188 HOMO: -6.41917 LUMO: 0.19320 factor:1 | 1 (-1.64422) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.99265 HOMO: -6.61237 LUMO: -0.04354 factor:1 | 1 (-1.33499) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85828 HOMO: -6.56339 LUMO: 0.36735 factor:1 | 1 (-1.20062) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.70827 HOMO: -6.54978 LUMO: 1.12655 factor:1 | 1 (-0.05061) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.33518 HOMO: -6.43277 LUMO: 1.17553 factor:1 | 1 (-1.67753) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.51894 HOMO: -6.29944 LUMO: 1.40955 factor:1 | 1 (-1.86129) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.62153 HOMO: -6.74842 LUMO: 0.74015 factor:1 | 1 (-1.96387) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.23651 HOMO: -6.15522 LUMO: 1.94289 factor:1 | 1 (-2.57885) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.95772 HOMO: -6.20147 LUMO: 1.40139 factor:1 | 1 (-2.30007) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.34931 HOMO: -6.41100 LUMO: 1.40139 factor:1 | 1 (-1.69165) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36041 HOMO: -6.74570 LUMO: 1.80956 factor:1 | 1 (-1.70275) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46777 HOMO: -6.60148 LUMO: -1.04764 factor:1 | 1 (-0.81011) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.24041 HOMO: -6.82734 LUMO: -0.83267 factor:1 | 1 (-1.58275) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14253 HOMO: -7.01782 LUMO: -0.32382 factor:1 | 1 (-1.48487) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50823 HOMO: -6.54434 LUMO: 0.11157 factor:1 | 1 (-0.85057) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.40899 HOMO: -6.53617 LUMO: 0.32926 factor:1 | 1 (-0.75133) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.57270 HOMO: -6.62597 LUMO: -0.60137 factor:1 | 1 (-2.91505) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.97362 HOMO: -6.60965 LUMO: -0.75376 factor:1 | 1 (-2.31596) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.83024 HOMO: -6.29399 LUMO: 0.06803 factor:1 | 1 (-2.17258) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.81624 HOMO: -6.60692 LUMO: -0.47076 factor:1 | 1 (-3.15859) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.40586 HOMO: -7.33891 LUMO: 0.39184 factor:1 | 1 (-0.74820) | 1 | 1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20250 HOMO: -6.60692 LUMO: 1.46125 factor:1 | 1 (-1.54484) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60290 HOMO: -6.21780 LUMO: 2.09256 factor:1 | 1 (-0.94524) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.39741 HOMO: -6.28311 LUMO: 1.80411 factor:1 | 1 (-1.73976) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.28195 HOMO: -6.51168 LUMO: 1.84765 factor:1 | 1 (-2.62429) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.46345 HOMO: -6.66951 LUMO: 2.01636 factor:1 | 1 (-2.80579) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.54953 HOMO: -6.75387 LUMO: 1.73881 factor:1 | 1 (-1.89187) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.28562 HOMO: -6.77291 LUMO: 1.89935 factor:1 | 1 (-2.62797) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.60164 HOMO: -6.36474 LUMO: 1.61091 factor:1 | 1 (-1.94398) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.41758 HOMO: -6.60420 LUMO: 1.40955 factor:1 | 1 (-1.75992) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.19841 HOMO: -6.81645 LUMO: 1.59731 factor:1 | 1 (-2.54075) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.83965 HOMO: -5.90215 LUMO: 2.12249 factor:1 | 1 (-2.18200) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.54482 HOMO: -6.26950 LUMO: 1.62996 factor:1 | 1 (-1.88716) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.94965 HOMO: -6.41100 LUMO: 1.80684 factor:1 | 1 (-1.29200) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.93248 HOMO: -6.64230 LUMO: 2.23405 factor:1 | 1 (-1.27483) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.04886 HOMO: -6.66951 LUMO: 2.21501 factor:1 | 1 (-1.39121) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05474 HOMO: -6.90897 LUMO: 2.00004 factor:1 | 1 (-1.39709) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.93931 HOMO: -6.61781 LUMO: 1.42043 factor:1 | 1 (-1.28166) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.19093 HOMO: -6.56611 LUMO: 1.60003 factor:1 | 1 (-2.53327) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.51129 HOMO: -6.70489 LUMO: 1.78779 factor:1 | 1 (-1.85364) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.51423 HOMO: -6.46815 LUMO: 1.59459 factor:1 | 1 (-1.85658) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69974 HOMO: -6.31304 LUMO: 1.36873 factor:1 | 1 (-1.04209) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.04418 HOMO: -6.22597 LUMO: 1.54833 factor:1 | 1 (-2.38652) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30291 HOMO: -5.63004 LUMO: 1.96466 factor:1 | 1 (-1.64525) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.92093 HOMO: -7.02598 LUMO: 1.79323 factor:1 | 1 (-2.26328) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.20886 HOMO: -6.78924 LUMO: 2.10888 factor:1 | 1 (-2.55120) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.36843 HOMO: -6.13345 LUMO: 2.07351 factor:1 | 1 (-2.71077) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.76123 HOMO: -6.46270 LUMO: -0.37552 factor:1 | 1 (-2.10358) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87215 HOMO: -6.51985 LUMO: -0.49525 factor:1 | 1 (-1.21450) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.87800 HOMO: -6.60965 LUMO: 1.90480 factor:1 | 1 (-2.22034) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.79724 HOMO: -6.51168 LUMO: 1.92112 factor:1 | 1 (-1.13959) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.73715 HOMO: -6.71305 LUMO: 1.91024 factor:1 | 1 (-2.07949) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.76556 HOMO: -6.86815 LUMO: 2.02997 factor:1 | 1 (-2.10790) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.84975 HOMO: -6.69944 LUMO: 1.95106 factor:1 | 1 (-2.19209) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69588 HOMO: -6.45182 LUMO: 1.66806 factor:1 | 1 (-1.03822) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.76787 HOMO: -6.44638 LUMO: 2.16058 factor:1 | 1 (-2.11022) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.51984 HOMO: -6.65591 LUMO: 1.95106 factor:1 | 1 (-1.86218) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.53419 HOMO: -6.35114 LUMO: 1.42316 factor:1 | 1 (-0.87653) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.00905 HOMO: -6.48719 LUMO: 1.59187 factor:1 | 1 (-1.35140) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.00541 HOMO: -7.05591 LUMO: 1.61908 factor:1 | 1 (-1.34775) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.38572 HOMO: -6.92258 LUMO: 1.87214 factor:1 | 1 (-0.72807) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.14954 HOMO: -5.85861 LUMO: 2.11705 factor:1 | -1 (0.50812) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.02753 HOMO: -6.27767 LUMO: 1.75513 factor:1 | 1 (-1.36988) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88380 HOMO: -6.16882 LUMO: 1.73881 factor:1 | 1 (-1.22615) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.32526 HOMO: -6.62053 LUMO: 1.39594 factor:1 | 1 (-0.66760) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01548 HOMO: -5.46405 LUMO: 1.68166 factor:1 | 1 (-1.35782) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.78048 HOMO: -6.39740 LUMO: 1.68711 factor:1 | 1 (-1.12282) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76238 HOMO: -6.99333 LUMO: 2.08439 factor:1 | 1 (-1.10473) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.13011 HOMO: -6.16882 LUMO: 1.71976 factor:1 | 1 (-2.47245) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.24772 HOMO: -7.19741 LUMO: 2.24766 factor:1 | 1 (-1.59007) | 1 | 1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.04143 HOMO: -6.77291 LUMO: 2.17691 factor:1 | 1 (-2.38377) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.98486 HOMO: -6.29944 LUMO: 2.16603 factor:1 | 1 (-1.32721) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91267 HOMO: -6.10079 LUMO: 1.83949 factor:1 | 1 (-1.25502) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.68166 HOMO: -6.63686 LUMO: 2.05990 factor:1 | 1 (-3.02400) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.12992 HOMO: -6.91713 LUMO: 1.87486 factor:1 | 1 (-2.47226) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.64881 HOMO: -6.63958 LUMO: 1.79323 factor:1 | 1 (-2.99116) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.10682 HOMO: -6.61781 LUMO: 1.70071 factor:1 | 1 (-2.44916) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.58945 HOMO: -6.20420 LUMO: 1.82861 factor:1 | 1 (-1.93179) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.58980 HOMO: -6.47903 LUMO: -2.16875 factor:1 | 1 (-1.93214) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.08772 HOMO: -6.53073 LUMO: 2.18235 factor:1 | 1 (-1.43007) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.69851 HOMO: -7.01782 LUMO: 1.72520 factor:1 | 1 (-2.04085) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.86062 HOMO: -6.66135 LUMO: -0.75648 factor:1 | 1 (-1.20296) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.84051 HOMO: -7.56749 LUMO: 0.22585 factor:1 | 1 (-1.18285) | 1 | 1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.09793 HOMO: -6.45182 LUMO: -0.71294 factor:1 | 1 (-1.44027) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.97599 HOMO: -6.31032 LUMO: -0.34286 factor:1 | 1 (-1.31834) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89485 HOMO: -6.41917 LUMO: 2.04085 factor:1 | 1 (-1.23719) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06778 HOMO: -6.61781 LUMO: 1.98915 factor:1 | 1 (-1.41012) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01877 HOMO: -5.86405 LUMO: 1.57282 factor:1 | 1 (-1.36111) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76984 HOMO: -6.44094 LUMO: 1.80956 factor:1 | 1 (-1.11218) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.92092 HOMO: -6.59060 LUMO: 2.08167 factor:1 | 1 (-1.26326) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.63718 HOMO: -6.20147 LUMO: 1.69799 factor:1 | 1 (-0.97953) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77204 HOMO: -6.50352 LUMO: -0.41361 factor:1 | 1 (-1.11439) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.35545 HOMO: -6.10896 LUMO: -0.55783 factor:1 | -1 (0.30221) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.85269 HOMO: -6.74842 LUMO: -0.56872 factor:1 | 1 (-2.19503) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.87609 HOMO: -6.59060 LUMO: -0.22041 factor:1 | 1 (-2.21844) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.77575 HOMO: -6.22052 LUMO: -0.60137 factor:1 | 1 (-0.11810) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.20256 HOMO: -6.65863 LUMO: 0.07891 factor:1 | 1 (-0.54491) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.25694 HOMO: -6.57427 LUMO: 1.71160 factor:1 | 1 (-2.59929) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.35542 HOMO: -5.84773 LUMO: 1.99459 factor:1 | 1 (-2.69776) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.85875 HOMO: -6.02188 LUMO: 1.91296 factor:1 | 1 (-3.20109) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.56982 HOMO: -6.17698 LUMO: 2.00004 factor:1 | 1 (-2.91216) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.27461 HOMO: -6.02732 LUMO: 1.90752 factor:1 | 1 (-1.61695) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88415 HOMO: -6.68584 LUMO: -0.50885 factor:1 | 1 (-1.22650) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.83476 HOMO: -6.61781 LUMO: -0.73471 factor:1 | 1 (-1.17711) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.31880 HOMO: -6.66407 LUMO: -0.79729 factor:1 | 1 (-1.66115) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87308 HOMO: -6.56339 LUMO: 0.23130 factor:1 | 1 (-1.21542) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81719 HOMO: -6.76747 LUMO: 0.08980 factor:1 | 1 (-1.15953) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.95030 HOMO: -6.70489 LUMO: -0.53334 factor:1 | 1 (-1.29265) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61810 HOMO: -7.28993 LUMO: 0.10885 factor:1 | 1 (-1.96044) | 1 | 1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.74714 HOMO: -6.22052 LUMO: 0.51974 factor:1 | 1 (-1.08949) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.44647 HOMO: -6.81645 LUMO: 0.25307 factor:1 | 1 (-2.78881) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.30192 HOMO: -6.80285 LUMO: 0.02721 factor:1 | 1 (-2.64427) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.81203 HOMO: -6.51441 LUMO: 0.08163 factor:1 | 1 (-2.15438) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96301 HOMO: -6.73482 LUMO: -0.77008 factor:1 | 1 (-1.30536) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.86390 HOMO: -6.29127 LUMO: -0.44355 factor:1 | 1 (-2.20624) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.20078 HOMO: -6.72938 LUMO: -0.64763 factor:1 | 1 (-2.54312) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.52580 HOMO: -6.49264 LUMO: -0.74559 factor:1 | 1 (-1.86814) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.54095 HOMO: -6.67223 LUMO: -0.55239 factor:1 | 1 (-1.88330) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.91030 HOMO: -6.33481 LUMO: 0.33198 factor:1 | 1 (-2.25264) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.91674 HOMO: -6.76475 LUMO: -0.25307 factor:1 | 1 (-2.25909) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.98486 HOMO: -6.65318 LUMO: 0.03810 factor:1 | 1 (-1.32721) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.29735 HOMO: -6.09263 LUMO: 0.21497 factor:1 | 1 (-2.63969) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.57720 HOMO: -6.32120 LUMO: -0.85444 factor:1 | 1 (-1.91955) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.52457 HOMO: -6.57155 LUMO: -0.67484 factor:1 | 1 (-1.86692) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.86817 HOMO: -6.53345 LUMO: -0.78913 factor:1 | 1 (-2.21052) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.42028 HOMO: -7.07768 LUMO: 0.28844 factor:1 | 1 (-0.76263) | 1 | 1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.51561 HOMO: -6.75114 LUMO: 0.18776 factor:1 | -1 (0.14204) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.07045 HOMO: -6.77019 LUMO: -0.12245 factor:1 | 1 (-0.41280) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.13884 HOMO: -6.43549 LUMO: 0.16327 factor:1 | 1 (-2.48119) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.15300 HOMO: -6.69400 LUMO: -0.16327 factor:1 | 1 (-1.49535) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.02703 HOMO: -6.38651 LUMO: -0.61770 factor:1 | 1 (-2.36938) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.13491 HOMO: -6.34297 LUMO: -0.33198 factor:1 | 1 (-1.47725) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.48446 HOMO: -7.51578 LUMO: 0.02177 factor:1 | 1 (-1.82681) | 1 | 1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.61857 HOMO: -6.47359 LUMO: -0.22585 factor:1 | 1 (-0.96092) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.75225 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-2.09460) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.53881 HOMO: -6.75659 LUMO: -0.57688 factor:1 | 1 (-1.88115) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.66946 HOMO: -6.73754 LUMO: -0.61226 factor:1 | 1 (-1.01180) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.39054 HOMO: -7.37429 LUMO: 0.31293 factor:1 | 1 (-0.73288) | 1 | 1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.98159 HOMO: -6.23413 LUMO: -0.90886 factor:1 | 1 (-2.32393) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87452 HOMO: -6.51985 LUMO: -0.68028 factor:1 | 1 (-1.21687) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36873 HOMO: -6.52257 LUMO: -0.77280 factor:1 | 1 (-1.71108) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80481 HOMO: -7.29537 LUMO: 0.31837 factor:1 | 1 (-1.14715) | 1 | 1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60643 HOMO: -6.08447 LUMO: 0.25851 factor:1 | 1 (-0.94878) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.65695 HOMO: -6.20964 LUMO: 0.13606 factor:1 | -1 (0.00071) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79799 HOMO: -6.49808 LUMO: -0.14150 factor:1 | 1 (-2.14034) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.08130 HOMO: -7.10761 LUMO: 0.28028 factor:1 | 1 (-1.42365) | 1 | 1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.63021 HOMO: -6.60965 LUMO: -0.62858 factor:1 | 1 (-1.97255) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.38437 HOMO: -6.40012 LUMO: -0.26939 factor:1 | -1 (0.27328) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.10922 HOMO: -6.65318 LUMO: -0.73199 factor:1 | 1 (-1.45156) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14674 HOMO: -6.51441 LUMO: -0.44899 factor:1 | 1 (-1.48909) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.17071 HOMO: -6.28583 LUMO: -0.48708 factor:1 | -1 (0.48695) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.93507 HOMO: -6.96884 LUMO: 0.19864 factor:1 | 1 (-1.27741) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23368 HOMO: -6.89809 LUMO: 0.34558 factor:1 | 1 (-1.57603) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17439 HOMO: -6.67495 LUMO: -0.15510 factor:1 | 1 (-1.51674) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.16519 HOMO: -7.34980 LUMO: 0.19864 factor:1 | 1 (-1.50754) | 1 | 1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.67919 HOMO: -6.71305 LUMO: -0.81634 factor:1 | -1 (0.97847) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57460 HOMO: -6.39468 LUMO: -0.47076 factor:1 | 1 (-0.91694) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.61140 HOMO: -6.31304 LUMO: 1.39594 factor:1 | -1 (0.04626) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.90023 HOMO: -6.57155 LUMO: 1.55105 factor:1 | -1 (0.75743) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88843 HOMO: -6.68312 LUMO: 1.69255 factor:1 | 1 (-1.23077) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.19913 HOMO: -6.61509 LUMO: 1.73881 factor:1 | 1 (-1.54147) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.75618 HOMO: -6.17971 LUMO: 1.90208 factor:1 | 1 (-1.09852) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.92394 HOMO: -6.53073 LUMO: 1.73337 factor:1 | 1 (-1.26628) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.42717 HOMO: -5.91303 LUMO: 1.90480 factor:1 | 1 (-0.76951) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.50350 HOMO: -6.42733 LUMO: 1.80139 factor:1 | -1 (0.15415) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.55722 HOMO: -6.78924 LUMO: 2.31569 factor:1 | -1 (0.10044) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.22442 HOMO: -6.04093 LUMO: 1.91568 factor:1 | -1 (0.43323) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.31417 HOMO: -6.90081 LUMO: 2.36739 factor:1 | -1 (0.34349) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52616 HOMO: -6.60965 LUMO: 2.18507 factor:1 | 1 (-0.86851) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.67061 HOMO: -6.75387 LUMO: 2.48712 factor:1 | 1 (-0.01295) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.37283 HOMO: -6.56883 LUMO: 1.71432 factor:1 | -1 (0.28482) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.92392 HOMO: -6.41644 LUMO: 1.72792 factor:1 | 1 (-0.26626) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.71513 HOMO: -6.92530 LUMO: 2.54426 factor:1 | 1 (-2.05748) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05575 HOMO: -6.41644 LUMO: 2.70209 factor:1 | 1 (-1.39809) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.81818 HOMO: -6.29671 LUMO: 2.14698 factor:1 | 1 (-2.16053) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.29227 HOMO: -6.29127 LUMO: 1.87486 factor:1 | 1 (-1.63462) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.08797 HOMO: -6.75931 LUMO: 2.78917 factor:1 | 1 (-1.43031) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.19039 HOMO: -6.40828 LUMO: 1.86942 factor:1 | 1 (-1.53274) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.74292 HOMO: -6.45726 LUMO: 1.97010 factor:1 | 1 (-2.08526) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14408 HOMO: -6.43277 LUMO: 1.22723 factor:1 | 1 (-1.48642) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14500 HOMO: -6.63414 LUMO: 1.62452 factor:1 | 1 (-1.48735) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80105 HOMO: -6.54162 LUMO: 2.16058 factor:1 | 1 (-1.14340) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.92046 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-0.26281) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.03678 HOMO: -6.20964 LUMO: 1.84221 factor:1 | 1 (-1.37913) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81645 HOMO: -6.58516 LUMO: 1.69799 factor:1 | 1 (-1.15880) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11678 HOMO: -6.44094 LUMO: 2.05446 factor:1 | 1 (-1.45913) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.27583 HOMO: -6.61509 LUMO: 2.16058 factor:1 | 1 (-1.61818) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11510 HOMO: -6.65591 LUMO: 1.69527 factor:1 | 1 (-1.45744) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.07253 HOMO: -5.55112 LUMO: 1.80411 factor:1 | -1 (0.58513) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.47333 HOMO: -6.68312 LUMO: 2.38100 factor:1 | 1 (-1.81568) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.31834 HOMO: -6.51168 LUMO: 2.14698 factor:1 | 1 (-1.66068) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81762 HOMO: -6.04637 LUMO: 1.48302 factor:1 | 1 (-1.15997) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.04264 HOMO: -6.81645 LUMO: -0.74287 factor:1 | 1 (-0.38499) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.27992 HOMO: -6.96884 LUMO: -0.97961 factor:1 | 1 (-1.62226) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.02307 HOMO: -6.45998 LUMO: 0.09796 factor:1 | 1 (-1.36541) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01436 HOMO: -6.44638 LUMO: 0.09524 factor:1 | 1 (-1.35671) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.10908 HOMO: -6.16338 LUMO: -0.54151 factor:1 | 1 (-1.45143) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62080 HOMO: -6.35930 LUMO: -0.47892 factor:1 | 1 (-0.96315) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.99608 HOMO: -6.65318 LUMO: -0.00272 factor:1 | 1 (-0.33843) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.32343 HOMO: -6.50080 LUMO: 0.14694 factor:1 | 1 (-1.66577) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45862 HOMO: -6.60420 LUMO: 0.94968 factor:1 | 1 (-0.80097) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23709 HOMO: -6.60148 LUMO: -0.77552 factor:1 | 1 (-1.57943) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57179 HOMO: -6.81645 LUMO: -1.05580 factor:1 | 1 (-0.91414) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62692 HOMO: -6.57971 LUMO: -0.82178 factor:1 | 1 (-0.96927) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.66762 HOMO: -6.09263 LUMO: -0.45171 factor:1 | 1 (-2.00997) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.33769 HOMO: -6.74298 LUMO: -0.61770 factor:1 | 1 (-1.68003) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.65840 HOMO: -6.72393 LUMO: 1.21091 factor:1 | 1 (-2.00074) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.84625 HOMO: -6.30488 LUMO: 1.70071 factor:1 | 1 (-1.18859) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.51625 HOMO: -6.38107 LUMO: 1.55649 factor:1 | 1 (-1.85859) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79691 HOMO: -6.17154 LUMO: 1.46669 factor:1 | 1 (-2.13925) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05637 HOMO: -6.86543 LUMO: 1.98643 factor:1 | 1 (-1.39872) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.95108 HOMO: -6.69944 LUMO: 1.65173 factor:1 | 1 (-2.29343) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.98037 HOMO: -6.77836 LUMO: 2.16331 factor:1 | 1 (-1.32272) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.92230 HOMO: -6.42189 LUMO: 2.36467 factor:1 | 1 (-2.26464) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.69157 HOMO: -7.00965 LUMO: 2.04358 factor:1 | 1 (-2.03392) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87253 HOMO: -6.36746 LUMO: 2.13881 factor:1 | 1 (-1.21488) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.53285 HOMO: -6.37835 LUMO: 1.89935 factor:1 | 1 (-1.87519) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01246 HOMO: -7.03959 LUMO: 1.27349 factor:1 | 1 (-1.35480) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.58158 HOMO: -6.67495 LUMO: -0.89253 factor:1 | 1 (-1.92393) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.74490 HOMO: -6.71849 LUMO: -0.97961 factor:1 | 1 (-2.08725) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.63998 HOMO: -6.47903 LUMO: 0.01633 factor:1 | 1 (-1.98232) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.26777 HOMO: -6.38379 LUMO: 0.01088 factor:1 | -1 (0.38988) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.63481 HOMO: -6.49536 LUMO: -0.55239 factor:1 | 1 (-1.97715) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64986 HOMO: -6.53345 LUMO: -0.53879 factor:1 | 1 (-0.99221) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06514 HOMO: -6.16610 LUMO: 2.15514 factor:1 | 1 (-1.40748) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.72399 HOMO: -6.35114 LUMO: 1.98643 factor:1 | 1 (-1.06633) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11714 HOMO: -6.43277 LUMO: 2.16058 factor:1 | 1 (-1.45948) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.13058 HOMO: -6.89809 LUMO: 2.20684 factor:1 | 1 (-1.47293) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96761 HOMO: -6.54434 LUMO: 1.93473 factor:1 | 1 (-1.30996) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06587 HOMO: -6.72938 LUMO: 2.03269 factor:1 | 1 (-1.40822) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.28364 HOMO: -6.90353 LUMO: 2.19868 factor:1 | 1 (-1.62599) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.22283 HOMO: -6.41372 LUMO: 2.02453 factor:1 | 1 (-1.56517) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30511 HOMO: -6.46543 LUMO: 1.90752 factor:1 | 1 (-1.64746) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.37377 HOMO: -6.55522 LUMO: 2.11977 factor:1 | 1 (-1.71611) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89798 HOMO: -6.28855 LUMO: 2.02181 factor:1 | 1 (-1.24032) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.44737 HOMO: -6.45726 LUMO: 1.52112 factor:1 | 1 (-1.78972) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.29942 HOMO: -6.37291 LUMO: 2.11705 factor:1 | -1 (0.35824) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89858 HOMO: -6.88448 LUMO: 2.24494 factor:1 | 1 (-1.24092) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52850 HOMO: -6.86271 LUMO: 2.41637 factor:1 | 1 (-0.87085) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.60209 HOMO: -6.69400 LUMO: 2.34562 factor:1 | -1 (0.05557) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.37032 HOMO: -6.18243 LUMO: 2.53882 factor:1 | 1 (-0.71267) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88788 HOMO: -6.61237 LUMO: 2.54154 factor:1 | 1 (-1.23023) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.38795 HOMO: -6.69672 LUMO: 2.16331 factor:1 | 1 (-1.73029) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.37668 HOMO: -6.33481 LUMO: 2.34018 factor:1 | 1 (-1.71902) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.67181 HOMO: -5.99739 LUMO: 2.37283 factor:1 | 1 (-2.01416) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85602 HOMO: -6.49808 LUMO: 2.47351 factor:1 | 1 (-1.19836) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.72486 HOMO: -6.22052 LUMO: 1.86398 factor:1 | 1 (-1.06720) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.78096 HOMO: -6.32665 LUMO: 2.28031 factor:1 | 1 (-2.12330) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.86829 HOMO: -5.98378 LUMO: 2.16331 factor:1 | 1 (-1.21063) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.64338 HOMO: -6.08991 LUMO: 2.30208 factor:1 | 1 (-1.98572) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59332 HOMO: -7.07224 LUMO: 1.55105 factor:1 | 1 (-0.93566) | 1 | 1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.65383 HOMO: -6.84638 LUMO: 1.76874 factor:1 | 1 (-1.99617) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.12617 HOMO: -6.68856 LUMO: 1.47758 factor:1 | 1 (-1.46852) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.99953 HOMO: -6.69672 LUMO: 1.71976 factor:1 | 1 (-1.34188) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.34129 HOMO: -6.86543 LUMO: 2.24766 factor:1 | 1 (-0.68363) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.00239 HOMO: -7.21646 LUMO: 1.71976 factor:1 | 1 (-1.34473) | 1 | 1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.44245 HOMO: -6.94162 LUMO: 2.21773 factor:1 | 1 (-1.78479) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.46150 HOMO: -6.34842 LUMO: 2.04358 factor:1 | 1 (-1.80384) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.68420 HOMO: -6.53345 LUMO: 1.96738 factor:1 | 1 (-2.02654) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.42294 HOMO: -6.34842 LUMO: 1.88303 factor:1 | 1 (-1.76528) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.43369 HOMO: -6.38651 LUMO: 2.08983 factor:1 | 1 (-1.77603) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.70158 HOMO: -6.01372 LUMO: 1.43676 factor:1 | 1 (-2.04393) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.46052 HOMO: -6.30216 LUMO: 1.41771 factor:1 | 1 (-1.80286) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64154 HOMO: -6.52801 LUMO: 1.77146 factor:1 | 1 (-0.98388) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20498 HOMO: -6.53617 LUMO: 1.72792 factor:1 | 1 (-1.54732) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.31916 HOMO: -6.56611 LUMO: 2.20412 factor:1 | 1 (-0.66151) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.65620 HOMO: -6.66679 LUMO: -0.72927 factor:1 | 1 (-0.99855) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.68316 HOMO: -6.85455 LUMO: -0.85444 factor:1 | 1 (-2.02551) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.87035 HOMO: -7.21646 LUMO: 0.27211 factor:1 | 1 (-2.21269) | 1 | 1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81776 HOMO: -6.57971 LUMO: -0.41361 factor:1 | 1 (-1.16010) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46567 HOMO: -7.03142 LUMO: -1.14288 factor:1 | 1 (-0.80801) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.11546 HOMO: -6.29944 LUMO: 0.06803 factor:1 | 1 (-0.45780) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.47336 HOMO: -6.47359 LUMO: 0.28028 factor:1 | 1 (-1.81571) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06737 HOMO: -6.42189 LUMO: 1.61364 factor:1 | 1 (-1.40971) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.73215 HOMO: -6.41100 LUMO: 1.80956 factor:1 | 1 (-1.07450) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58045 HOMO: -6.83278 LUMO: 1.83949 factor:1 | 1 (-0.92279) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.13409 HOMO: -6.78380 LUMO: -0.76192 factor:1 | 1 (-1.47644) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.21979 HOMO: -6.95795 LUMO: 2.13609 factor:1 | 1 (-0.56213) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23001 HOMO: -6.57155 LUMO: 1.89119 factor:1 | 1 (-1.57236) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91504 HOMO: -6.65591 LUMO: 1.93745 factor:1 | 1 (-1.25738) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60785 HOMO: -6.44638 LUMO: 2.26943 factor:1 | 1 (-0.95019) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50901 HOMO: -5.88038 LUMO: 1.90480 factor:1 | 1 (-1.85135) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.43694 HOMO: -6.22052 LUMO: 2.17691 factor:1 | -1 (0.22071) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64148 HOMO: -6.04637 LUMO: 2.23950 factor:1 | 1 (-0.98383) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06745 HOMO: -6.44366 LUMO: 2.24766 factor:1 | 1 (-1.40979) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.52240 HOMO: -6.81917 LUMO: 2.08439 factor:1 | 1 (-1.86474) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.99615 HOMO: -6.48447 LUMO: 2.28576 factor:1 | 1 (-2.33849) | -1 | -1 |
| G: -6694.29196 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.96638 HOMO: -6.54434 LUMO: 1.99187 factor:1 | 1 (-2.30872) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.67364 HOMO: -6.17698 LUMO: -0.65852 factor:1 | 1 (-2.01598) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.03794 HOMO: -6.08174 LUMO: -0.58504 factor:1 | 1 (-2.38029) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.34053 HOMO: -6.55250 LUMO: -0.86804 factor:1 | 1 (-2.68288) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.76482 HOMO: -6.57699 LUMO: -0.89525 factor:1 | 1 (-2.10717) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.23849 HOMO: -6.63141 LUMO: -1.04220 factor:1 | 1 (-2.58084) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.63066 HOMO: -6.69128 LUMO: -0.76736 factor:1 | 1 (-2.97301) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.26897 HOMO: -6.25318 LUMO: -1.03131 factor:1 | 1 (-2.61131) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76568 HOMO: -6.69944 LUMO: 0.01905 factor:1 | 1 (-1.10802) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.55027 HOMO: -6.28583 LUMO: 0.38368 factor:1 | 1 (-0.89262) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58080 HOMO: -6.90081 LUMO: -0.83811 factor:1 | 1 (-0.92315) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.98884 HOMO: -6.78380 LUMO: -0.10068 factor:1 | 1 (-0.33119) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79388 HOMO: -6.30488 LUMO: -0.98505 factor:1 | 1 (-2.13623) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89009 HOMO: -6.29671 LUMO: -1.79051 factor:1 | 1 (-1.23243) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.38101 HOMO: -6.76747 LUMO: -0.22041 factor:1 | 1 (-1.72335) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.28739 HOMO: -6.22597 LUMO: -0.94968 factor:1 | 1 (-2.62974) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.73369 HOMO: -6.73482 LUMO: 0.05987 factor:1 | 1 (-2.07604) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.37131 HOMO: -6.28855 LUMO: 0.34831 factor:1 | 1 (-2.71366) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.40278 HOMO: -6.69400 LUMO: 0.25307 factor:1 | 1 (-1.74512) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.78635 HOMO: -6.70216 LUMO: 0.61226 factor:1 | 1 (-2.12869) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.00843 HOMO: -6.70216 LUMO: 0.17415 factor:1 | 1 (-1.35077) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85730 HOMO: -6.70761 LUMO: 0.24762 factor:1 | 1 (-1.19964) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.74374 HOMO: -6.68856 LUMO: -0.84900 factor:1 | 1 (-1.08609) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.49966 HOMO: -6.71033 LUMO: -0.38640 factor:1 | 1 (-0.84200) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52156 HOMO: -6.24501 LUMO: -0.09252 factor:1 | 1 (-0.86391) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69710 HOMO: -6.81645 LUMO: -0.07347 factor:1 | 1 (-1.03945) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.56265 HOMO: -6.49536 LUMO: 0.09796 factor:1 | 1 (-0.90500) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.08860 HOMO: -6.71033 LUMO: -0.26395 factor:1 | 1 (-0.43095) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91175 HOMO: -6.70489 LUMO: -0.09252 factor:1 | 1 (-1.25409) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.04214 HOMO: -6.23685 LUMO: 0.39729 factor:1 | 1 (-1.38449) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70782 HOMO: -6.69400 LUMO: -0.05442 factor:1 | 1 (-1.05017) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52477 HOMO: -6.36202 LUMO: 0.09796 factor:1 | 1 (-0.86712) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.56113 HOMO: -6.54978 LUMO: 0.15510 factor:1 | 1 (-0.90347) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.96860 HOMO: -6.77836 LUMO: 0.25851 factor:1 | 1 (-0.31094) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.39513 HOMO: -5.70623 LUMO: 0.73471 factor:1 | 1 (-1.73747) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30302 HOMO: -5.58378 LUMO: 0.89253 factor:1 | 1 (-1.64536) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.71576 HOMO: -5.68718 LUMO: 0.87893 factor:1 | 1 (-2.05811) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.99762 HOMO: -5.10486 LUMO: 1.11567 factor:1 | 1 (-2.33996) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.71475 HOMO: -4.59328 LUMO: 1.27621 factor:1 | 1 (-3.05709) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.00222 HOMO: -4.45450 LUMO: 1.82044 factor:1 | 1 (-2.34456) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.56903 HOMO: -4.64226 LUMO: 1.70615 factor:1 | 1 (-2.91137) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14680 HOMO: -5.04227 LUMO: 1.04492 factor:1 | 1 (-1.48914) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.72518 HOMO: -4.85723 LUMO: 0.93607 factor:1 | 1 (-2.06752) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.71633 HOMO: -4.72934 LUMO: 1.00410 factor:1 | 1 (-2.05868) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50887 HOMO: -4.56335 LUMO: 1.56738 factor:1 | 1 (-1.85122) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79271 HOMO: -5.48854 LUMO: 0.33198 factor:1 | 1 (-2.13506) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.18244 HOMO: -4.97424 LUMO: 1.33608 factor:1 | 1 (-2.52478) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.10341 HOMO: -4.60145 LUMO: 1.74697 factor:1 | 1 (-2.44576) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.09871 HOMO: -5.60010 LUMO: 0.74831 factor:1 | 1 (-2.44105) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.03749 HOMO: -5.66541 LUMO: 0.66668 factor:1 | 1 (-1.37983) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06182 HOMO: -6.50080 LUMO: 0.07075 factor:1 | 1 (-1.40416) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.56015 HOMO: -5.79603 LUMO: 0.22313 factor:1 | 1 (-0.90249) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.71044 HOMO: -4.68036 LUMO: 1.29798 factor:1 | 1 (-1.05278) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06837 HOMO: -4.84363 LUMO: 1.34424 factor:1 | 1 (-1.41072) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.00930 HOMO: -4.62321 LUMO: 1.82861 factor:1 | 1 (-1.35164) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58905 HOMO: -5.83684 LUMO: 0.82178 factor:1 | 1 (-0.93139) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62431 HOMO: -5.27629 LUMO: 0.57960 factor:1 | 1 (-0.96666) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77846 HOMO: -5.15928 LUMO: -2.96876 factor:1 | 1 (-1.12081) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.12867 HOMO: -5.08853 LUMO: 0.89253 factor:1 | 1 (-2.47101) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.09098 HOMO: -6.42461 LUMO: 0.04354 factor:1 | 1 (-2.43332) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.49044 HOMO: -6.42733 LUMO: -0.00544 factor:1 | 1 (-2.83279) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.65080 HOMO: -5.87494 LUMO: 0.69933 factor:1 | 1 (-2.99314) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.52835 HOMO: -5.07492 LUMO: 1.02587 factor:1 | 1 (-2.87069) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.36824 HOMO: -4.44362 LUMO: 1.99187 factor:1 | 1 (-2.71058) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.68802 HOMO: -5.82052 LUMO: 0.43810 factor:1 | 1 (-3.03037) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.67687 HOMO: -5.75793 LUMO: 0.76464 factor:1 | 1 (-3.01921) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.73821 HOMO: -5.09669 LUMO: 0.72382 factor:1 | 1 (-2.08056) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.48190 HOMO: -6.75387 LUMO: -2.02453 factor:1 | 1 (-2.82424) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.88447 HOMO: -5.02322 LUMO: 1.14832 factor:1 | 1 (-2.22682) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.04639 HOMO: -5.75521 LUMO: 0.73471 factor:1 | 1 (-1.38873) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05444 HOMO: -5.89943 LUMO: 0.54967 factor:1 | 1 (-1.39679) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58086 HOMO: -5.80147 LUMO: 0.72382 factor:1 | 1 (-0.92320) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68521 HOMO: -6.16066 LUMO: 0.39457 factor:1 | 1 (-1.02756) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.53095 HOMO: -5.98650 LUMO: 0.76736 factor:1 | 1 (-0.87330) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.34662 HOMO: -4.74839 LUMO: 1.88847 factor:1 | 1 (-0.68897) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17540 HOMO: -5.62459 LUMO: 0.26939 factor:1 | 1 (-1.51774) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.17830 HOMO: -4.88172 LUMO: 1.30070 factor:1 | 1 (-2.52065) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.32792 HOMO: -5.09397 LUMO: 0.98505 factor:1 | 1 (-1.67026) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.05574 HOMO: -6.50080 LUMO: -0.28300 factor:1 | 1 (-2.39809) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.31724 HOMO: -5.04227 LUMO: 1.49935 factor:1 | 1 (-2.65959) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.46084 HOMO: -5.22731 LUMO: 0.88437 factor:1 | 1 (-1.80319) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.31924 HOMO: -4.95519 LUMO: 1.25717 factor:1 | 1 (-1.66158) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.01220 HOMO: -4.61233 LUMO: 1.27621 factor:1 | 1 (-2.35455) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50452 HOMO: -4.70757 LUMO: 1.63813 factor:1 | 1 (-1.84686) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.66818 HOMO: -4.85179 LUMO: 1.11839 factor:1 | 1 (-1.01052) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.72578 HOMO: -4.97696 LUMO: 1.00138 factor:1 | 1 (-1.06813) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.63538 HOMO: -5.64636 LUMO: 0.81090 factor:1 | 1 (-1.97772) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.04173 HOMO: -4.37831 LUMO: 1.90208 factor:1 | 1 (-2.38407) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79759 HOMO: -4.67764 LUMO: 1.54561 factor:1 | 1 (-2.13993) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76706 HOMO: -5.87766 LUMO: 0.42994 factor:1 | 1 (-1.10941) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59792 HOMO: -6.03821 LUMO: 0.32382 factor:1 | 1 (-0.94026) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.70390 HOMO: -5.99739 LUMO: 0.69389 factor:1 | 1 (-2.04624) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.78368 HOMO: -6.43821 LUMO: 0.15238 factor:1 | 1 (-2.12603) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.42952 HOMO: -6.63414 LUMO: -0.07347 factor:1 | 1 (-1.77187) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.76266 HOMO: -6.50080 LUMO: 0.10068 factor:1 | 1 (-0.10501) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.66984 HOMO: -6.49264 LUMO: 0.19592 factor:1 | 1 (-1.01218) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.37815 HOMO: -5.83956 LUMO: 0.12517 factor:1 | 1 (-1.72049) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.51881 HOMO: -6.50896 LUMO: 0.19048 factor:1 | 1 (-0.86116) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.91049 HOMO: -6.56611 LUMO: 0.04898 factor:1 | 1 (-2.25283) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.07384 HOMO: -6.68040 LUMO: -0.08436 factor:1 | 1 (-2.41618) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45810 HOMO: -6.73754 LUMO: -0.08708 factor:1 | 1 (-0.80045) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61617 HOMO: -6.80285 LUMO: -0.10612 factor:1 | 1 (-1.95851) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.04017 HOMO: -6.35658 LUMO: 0.02177 factor:1 | 1 (-0.38251) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.30123 HOMO: -5.74160 LUMO: 0.14694 factor:1 | 1 (-0.64358) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.87318 HOMO: -4.78376 LUMO: 0.92791 factor:1 | 1 (-2.21552) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.45252 HOMO: -5.90215 LUMO: 0.36463 factor:1 | 1 (-1.79486) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.04880 HOMO: -4.99329 LUMO: 0.85988 factor:1 | 1 (-2.39115) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.59189 HOMO: -4.93887 LUMO: 1.33608 factor:1 | 1 (-1.93424) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.77973 HOMO: -5.19193 LUMO: 0.50341 factor:1 | 1 (-2.12208) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17442 HOMO: -6.64502 LUMO: -1.98643 factor:1 | 1 (-1.51676) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57982 HOMO: -5.15384 LUMO: 0.94968 factor:1 | 1 (-0.92217) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68630 HOMO: -6.31032 LUMO: 0.08436 factor:1 | 1 (-1.02864) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.45831 HOMO: -4.88716 LUMO: 0.82995 factor:1 | 1 (-1.80066) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.28711 HOMO: -5.57017 LUMO: 0.19320 factor:1 | 1 (-0.62945) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58747 HOMO: -4.92254 LUMO: 0.93879 factor:1 | 1 (-0.92981) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.86653 HOMO: -4.77288 LUMO: 1.60003 factor:1 | 1 (-0.20887) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88976 HOMO: -4.97696 LUMO: 0.89798 factor:1 | 1 (-1.23210) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.37310 HOMO: -5.00690 LUMO: 1.14288 factor:1 | 1 (-0.71544) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96312 HOMO: -4.88444 LUMO: 1.48574 factor:1 | 1 (-1.30547) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.02123 HOMO: -5.03955 LUMO: 1.51023 factor:1 | 1 (-0.36357) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.71464 HOMO: -5.22459 LUMO: 0.99049 factor:1 | 1 (-0.05698) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69629 HOMO: -5.29534 LUMO: 0.96056 factor:1 | 1 (-1.03863) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.92206 HOMO: -5.35520 LUMO: 0.68301 factor:1 | 1 (-1.26440) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27024 HOMO: -5.27357 LUMO: 1.18642 factor:1 | 1 (-0.61258) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.98675 HOMO: -5.79875 LUMO: 0.61770 factor:1 | 1 (-0.32909) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69751 HOMO: -7.64640 LUMO: -2.45175 factor:1 | 1 (-1.03986) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05039 HOMO: -7.46953 LUMO: -1.29798 factor:1 | 1 (-1.39273) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.62327 HOMO: -7.95389 LUMO: -0.37280 factor:1 | 1 (-1.96561) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88383 HOMO: -7.23279 LUMO: -1.19186 factor:1 | 1 (-1.22617) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.55737 HOMO: -7.14299 LUMO: -1.12927 factor:1 | 1 (-0.89972) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.26983 HOMO: -6.93074 LUMO: 0.31565 factor:1 | 1 (-0.61217) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59345 HOMO: -6.63141 LUMO: 0.28028 factor:1 | 1 (-0.93580) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46572 HOMO: -7.10489 LUMO: -1.07213 factor:1 | 1 (-0.80807) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70061 HOMO: -7.00693 LUMO: -0.69389 factor:1 | 1 (-1.04296) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81909 HOMO: -8.50356 LUMO: -1.79595 factor:1 | 1 (-1.16144) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.02703 HOMO: -7.79334 LUMO: -2.33746 factor:1 | 1 (-2.36938) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.29177 HOMO: -7.24367 LUMO: -0.85172 factor:1 | 1 (-2.63412) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61236 HOMO: -7.94028 LUMO: -0.20136 factor:1 | 1 (-1.95470) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36473 HOMO: -7.22462 LUMO: 0.84627 factor:1 | 1 (-1.70708) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77212 HOMO: -6.54978 LUMO: 0.34831 factor:1 | 1 (-1.11447) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.24160 HOMO: -6.86815 LUMO: 0.32109 factor:1 | 1 (-1.58395) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.66635 HOMO: -7.17564 LUMO: -1.28438 factor:1 | 1 (-1.00870) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27451 HOMO: -7.03142 LUMO: -1.12655 factor:1 | 1 (-0.61685) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05463 HOMO: -7.39878 LUMO: 0.15783 factor:1 | 1 (-1.39698) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58706 HOMO: -7.25728 LUMO: 0.42178 factor:1 | 1 (-0.92940) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81041 HOMO: -6.86543 LUMO: 0.93879 factor:1 | 1 (-1.15276) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.75579 HOMO: -7.09673 LUMO: -0.69661 factor:1 | 1 (-2.09813) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.23822 HOMO: -7.74708 LUMO: 0.01088 factor:1 | 1 (-2.58056) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.67630 HOMO: -6.80557 LUMO: 0.46531 factor:1 | 1 (-2.01865) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.47872 HOMO: -7.29265 LUMO: 1.31975 factor:1 | 1 (-1.82107) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.69481 HOMO: -6.93618 LUMO: 0.29388 factor:1 | 1 (-2.03715) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27119 HOMO: -6.53073 LUMO: 0.71022 factor:1 | 1 (-0.61354) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.04114 HOMO: -6.41917 LUMO: -1.24084 factor:1 | 1 (-0.38349) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.31160 HOMO: -6.67495 LUMO: -1.09118 factor:1 | 1 (-0.65394) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.42537 HOMO: -6.97156 LUMO: -0.53606 factor:1 | 1 (-0.76771) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.24509 HOMO: -6.85183 LUMO: -0.45715 factor:1 | 1 (-0.58744) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.26678 HOMO: -7.12666 LUMO: -0.67484 factor:1 | 1 (-0.60913) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.22085 HOMO: -7.49946 LUMO: -0.14694 factor:1 | 1 (-0.56319) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79440 HOMO: -7.44231 LUMO: 0.58232 factor:1 | 1 (-2.13675) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80168 HOMO: -7.36340 LUMO: -0.68301 factor:1 | 1 (-1.14402) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.37692 HOMO: -6.13073 LUMO: -0.54967 factor:1 | 1 (-2.71926) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.64773 HOMO: -7.81511 LUMO: -0.06531 factor:1 | 1 (-1.99008) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.39358 HOMO: -7.26816 LUMO: -1.02587 factor:1 | 1 (-1.73592) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.70537 HOMO: -7.98110 LUMO: -0.17960 factor:1 | 1 (-2.04771) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.38289 HOMO: -7.44776 LUMO: -1.00954 factor:1 | 1 (-0.72524) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.43651 HOMO: -7.47769 LUMO: -1.02859 factor:1 | -1 (0.22115) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.10047 HOMO: -6.75659 LUMO: 0.39457 factor:1 | 1 (-0.44281) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.40044 HOMO: -6.71849 LUMO: 0.36735 factor:1 | 1 (-1.74278) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.56842 HOMO: -7.64096 LUMO: -1.43948 factor:1 | 1 (-0.91077) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.37214 HOMO: -7.83144 LUMO: -1.36601 factor:1 | 1 (-0.71449) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.12261 HOMO: -7.19469 LUMO: 0.35103 factor:1 | 1 (-1.46495) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.18441 HOMO: -7.03414 LUMO: 0.20409 factor:1 | 1 (-0.52676) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.38574 HOMO: -7.22734 LUMO: 0.31293 factor:1 | 1 (-1.72809) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.49870 HOMO: -6.93618 LUMO: 0.56055 factor:1 | 1 (-0.84105) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.32858 HOMO: -6.94707 LUMO: -0.88709 factor:1 | 1 (-0.67092) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11670 HOMO: -6.86543 LUMO: -0.83267 factor:1 | 1 (-1.45905) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.55808 HOMO: -6.82189 LUMO: -1.15376 factor:1 | 1 (-0.90042) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.15156 HOMO: -6.65046 LUMO: -0.46531 factor:1 | 1 (-1.49391) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.25738 HOMO: -6.52529 LUMO: 0.20953 factor:1 | -1 (1.40027) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.97332 HOMO: -6.80557 LUMO: 0.44355 factor:1 | -1 (0.68434) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.61589 HOMO: -6.93074 LUMO: -0.81634 factor:1 | -1 (1.04176) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.92113 HOMO: -7.43143 LUMO: -0.45987 factor:1 | 1 (-1.26348) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45740 HOMO: -7.07224 LUMO: -0.68028 factor:1 | 1 (-0.79974) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.13640 HOMO: -6.68040 LUMO: -0.71566 factor:1 | 1 (-1.47875) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.99145 HOMO: -6.26406 LUMO: -1.09934 factor:1 | 1 (-1.33379) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.61928 HOMO: -5.94569 LUMO: -0.72110 factor:1 | 1 (-0.96162) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.36964 HOMO: -6.12256 LUMO: -0.42178 factor:1 | 1 (-0.71199) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.02307 HOMO: -6.09807 LUMO: 0.11429 factor:1 | 1 (-1.36541) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.13224 HOMO: -7.35252 LUMO: -0.55783 factor:1 | 1 (-1.47459) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.04271 HOMO: -7.57837 LUMO: -0.76736 factor:1 | 1 (-1.38506) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.10205 HOMO: -6.16066 LUMO: 0.01905 factor:1 | -1 (0.55560) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76168 HOMO: -6.13345 LUMO: -0.41906 factor:1 | 1 (-1.10402) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.64851 HOMO: -6.10351 LUMO: -0.33742 factor:1 | -1 (0.00914) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.11824 HOMO: -7.24639 LUMO: -0.51702 factor:1 | 1 (-2.46059) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23907 HOMO: -6.98244 LUMO: -1.82044 factor:1 | 1 (-1.58142) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.98208 HOMO: -6.37563 LUMO: -1.67622 factor:1 | 1 (-2.32442) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.07852 HOMO: -5.79058 LUMO: -2.55243 factor:1 | 1 (-1.42087) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.09800 HOMO: -6.34025 LUMO: -0.27483 factor:1 | 1 (-2.44034) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.22089 HOMO: -6.05453 LUMO: -0.51157 factor:1 | 1 (-1.56324) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.69873 HOMO: -7.53755 LUMO: -0.38912 factor:1 | 1 (-2.04107) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96549 HOMO: -7.00421 LUMO: -0.50885 factor:1 | 1 (-1.30783) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.20243 HOMO: -7.52123 LUMO: -0.37552 factor:1 | 1 (-0.54477) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.80620 HOMO: -6.70489 LUMO: -1.04764 factor:1 | 1 (-0.14855) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58086 HOMO: -7.06408 LUMO: -1.16737 factor:1 | 1 (-0.92320) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.93403 HOMO: -6.71849 LUMO: -1.02315 factor:1 | 1 (-1.27638) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.57238 HOMO: -6.16610 LUMO: -0.50885 factor:1 | 1 (-1.91473) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.82689 HOMO: -6.48447 LUMO: 0.07619 factor:1 | 1 (-2.16924) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14043 HOMO: -7.06135 LUMO: 0.09796 factor:1 | 1 (-1.48278) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80535 HOMO: -6.47359 LUMO: 0.22585 factor:1 | 1 (-1.14769) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.70413 HOMO: -6.10896 LUMO: -0.62314 factor:1 | 1 (-0.04648) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.90834 HOMO: -6.88176 LUMO: -0.96600 factor:1 | 1 (-1.25069) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.22364 HOMO: -6.67495 LUMO: 0.21769 factor:1 | 1 (-1.56599) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.76828 HOMO: -6.84911 LUMO: 0.38368 factor:1 | -1 (0.88938) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.34349 HOMO: -6.83550 LUMO: 1.29798 factor:1 | 1 (-0.68584) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.94209 HOMO: -6.67495 LUMO: 1.46941 factor:1 | 1 (-1.28443) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.09998 HOMO: -6.81917 LUMO: 1.30887 factor:1 | 1 (-0.44232) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.76236 HOMO: -6.56611 LUMO: 0.66396 factor:1 | 1 (-0.10471) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.63512 HOMO: -6.76203 LUMO: 0.60137 factor:1 | 1 (-0.97746) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69259 HOMO: -6.55794 LUMO: 0.34286 factor:1 | 1 (-1.03493) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58951 HOMO: -6.83550 LUMO: 0.35919 factor:1 | 1 (-0.93185) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.49040 HOMO: -7.17836 LUMO: 0.63130 factor:1 | 1 (-0.83275) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.90218 HOMO: -6.29944 LUMO: -0.69389 factor:1 | 1 (-0.24452) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85215 HOMO: -7.06680 LUMO: -0.95784 factor:1 | 1 (-1.19450) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.20697 HOMO: -6.84638 LUMO: -0.87076 factor:1 | 1 (-0.54932) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.07647 HOMO: -6.96339 LUMO: -1.05308 factor:1 | 1 (-0.41881) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62143 HOMO: -6.75387 LUMO: -1.04220 factor:1 | 1 (-0.96377) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.74631 HOMO: -6.71849 LUMO: -0.84355 factor:1 | 1 (-0.08865) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01597 HOMO: -7.16748 LUMO: 0.51702 factor:1 | 1 (-1.35831) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.95011 HOMO: -6.92530 LUMO: 0.71566 factor:1 | 1 (-1.29246) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76018 HOMO: -7.11034 LUMO: 0.01905 factor:1 | 1 (-1.10252) | 1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.89576 HOMO: -6.79468 LUMO: 0.77008 factor:1 | -1 (0.76189) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60935 HOMO: -6.52801 LUMO: 0.98233 factor:1 | 1 (-0.95169) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96617 HOMO: -6.76475 LUMO: 0.53334 factor:1 | 1 (-1.30851) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.09541 HOMO: -5.29261 LUMO: 0.57416 factor:1 | -1 (0.56224) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.08568 HOMO: -6.57971 LUMO: 0.12789 factor:1 | 1 (-1.42803) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.67724 HOMO: -6.99333 LUMO: 0.51430 factor:1 | 1 (-1.01958) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.58516 HOMO: -6.41917 LUMO: 0.19048 factor:1 | -1 (0.07249) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.33628 HOMO: -6.16066 LUMO: 1.77146 factor:1 | 1 (-0.67862) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.51972 HOMO: -6.90353 LUMO: 1.65717 factor:1 | -1 (0.13793) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.53351 HOMO: -5.94569 LUMO: 1.29526 factor:1 | 1 (-0.87585) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45198 HOMO: -6.60420 LUMO: 1.33880 factor:1 | 1 (-0.79433) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.37565 HOMO: -6.23957 LUMO: 0.09524 factor:1 | 1 (-0.71800) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.90829 HOMO: -6.80013 LUMO: 1.34696 factor:1 | 1 (-1.25064) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.67283 HOMO: -7.53483 LUMO: -1.52384 factor:1 | 1 (-1.01518) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96062 HOMO: -7.62463 LUMO: -1.65717 factor:1 | 1 (-1.30296) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.75634 HOMO: -7.62463 LUMO: -1.61364 factor:1 | 1 (-1.09869) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.98609 HOMO: -8.04096 LUMO: -1.66806 factor:1 | 1 (-1.32843) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.78306 HOMO: -7.18381 LUMO: -1.17553 factor:1 | 1 (-1.12541) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.74805 HOMO: -7.69538 LUMO: -1.36601 factor:1 | 1 (-0.09040) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.53781 HOMO: -7.95117 LUMO: -1.48302 factor:1 | 1 (-0.88015) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.55896 HOMO: -6.98516 LUMO: 0.35919 factor:1 | -1 (0.09870) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.21162 HOMO: -7.91579 LUMO: -0.32109 factor:1 | 1 (-0.55397) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.28574 HOMO: -6.75659 LUMO: -0.03537 factor:1 | -1 (1.37192) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.93187 HOMO: -7.78518 LUMO: -2.36467 factor:1 | -1 (0.72578) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.64926 HOMO: -7.96477 LUMO: -2.75651 factor:1 | -1 (1.00840) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77901 HOMO: -7.60286 LUMO: -2.35106 factor:1 | 1 (-1.12135) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57408 HOMO: -7.38245 LUMO: -1.21635 factor:1 | 1 (-0.91643) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.82932 HOMO: -7.91579 LUMO: -1.50479 factor:1 | 1 (-1.17167) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.92955 HOMO: -8.07362 LUMO: -0.28028 factor:1 | 1 (-0.27190) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.78731 HOMO: -7.38245 LUMO: -1.15921 factor:1 | 1 (-1.12965) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69109 HOMO: -7.18653 LUMO: -0.94968 factor:1 | 1 (-1.03343) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.56336 HOMO: -6.88448 LUMO: 0.38096 factor:1 | 1 (-0.90570) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.97395 HOMO: -6.97972 LUMO: 0.43266 factor:1 | 1 (-1.31630) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89267 HOMO: -6.88992 LUMO: -0.43538 factor:1 | 1 (-1.23502) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.95294 HOMO: -7.97021 LUMO: -0.17143 factor:1 | 1 (-1.29529) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.19138 HOMO: -6.92530 LUMO: 0.77280 factor:1 | 1 (-0.53372) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.25718 HOMO: -7.89674 LUMO: -0.09796 factor:1 | -1 (0.40047) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.36872 HOMO: -7.02870 LUMO: 0.88709 factor:1 | 1 (-0.71106) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.50075 HOMO: -6.78380 LUMO: 0.22041 factor:1 | -1 (0.15690) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46605 HOMO: -7.24911 LUMO: -0.82178 factor:1 | 1 (-0.80840) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.27861 HOMO: -6.77019 LUMO: 0.52790 factor:1 | 1 (-1.62096) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.33692 HOMO: -8.56070 LUMO: -1.83405 factor:1 | 1 (-1.67927) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62004 HOMO: -7.74164 LUMO: -2.36195 factor:1 | 1 (-0.96239) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61992 HOMO: -7.39878 LUMO: -2.41637 factor:1 | 1 (-1.96227) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.92252 HOMO: -7.61647 LUMO: -2.34018 factor:1 | 1 (-1.26487) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.02664 HOMO: -6.93346 LUMO: -0.57688 factor:1 | 1 (-0.36899) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.61884 HOMO: -6.85183 LUMO: -1.00410 factor:1 | 1 (-0.96119) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.97738 HOMO: -7.18925 LUMO: -1.12655 factor:1 | 1 (-1.31973) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.94568 HOMO: -6.85183 LUMO: -1.60275 factor:1 | 1 (-1.28802) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.38009 HOMO: -7.51578 LUMO: 0.12517 factor:1 | 1 (-0.72244) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.65612 HOMO: -7.36068 LUMO: 0.05714 factor:1 | 1 (-0.99847) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.54224 HOMO: -7.49674 LUMO: 0.18776 factor:1 | 1 (-0.88459) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.95695 HOMO: -7.09401 LUMO: -1.24900 factor:1 | 1 (-0.29930) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80823 HOMO: -7.22462 LUMO: -1.61364 factor:1 | 1 (-1.15058) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.24216 HOMO: -7.74436 LUMO: -0.18776 factor:1 | 1 (-0.58450) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.97998 HOMO: -7.35252 LUMO: 0.75376 factor:1 | 1 (-2.32233) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17336 HOMO: -7.75252 LUMO: 0.00816 factor:1 | 1 (-1.51570) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.98513 HOMO: -7.06680 LUMO: 0.24490 factor:1 | 1 (-2.32747) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01308 HOMO: -7.49129 LUMO: 0.14150 factor:1 | 1 (-1.35543) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23692 HOMO: -6.90625 LUMO: -1.11295 factor:1 | 1 (-1.57927) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.04978 HOMO: -6.78380 LUMO: -0.93063 factor:1 | 1 (-2.39213) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.55709 HOMO: -7.79878 LUMO: 0.30477 factor:1 | 1 (-1.89944) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91942 HOMO: -7.87498 LUMO: 0.61770 factor:1 | 1 (-1.26176) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.10855 HOMO: -7.23823 LUMO: 0.30205 factor:1 | 1 (-0.45089) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.02729 HOMO: -7.67633 LUMO: 0.13061 factor:1 | 1 (-1.36963) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.94466 HOMO: -7.79606 LUMO: 0.34558 factor:1 | 1 (-2.28701) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.56419 HOMO: -6.66135 LUMO: -2.60141 factor:1 | 1 (-1.90654) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.97931 HOMO: -7.03142 LUMO: 0.50885 factor:1 | 1 (-1.32166) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.94088 HOMO: -7.05591 LUMO: -0.06531 factor:1 | 1 (-2.28323) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.57943 HOMO: -7.45592 LUMO: -1.39594 factor:1 | 1 (-1.92178) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.94750 HOMO: -7.22462 LUMO: -1.10478 factor:1 | 1 (-1.28985) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.60166 HOMO: -8.14709 LUMO: -0.55783 factor:1 | 1 (-1.94401) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.09284 HOMO: -7.22190 LUMO: -1.14560 factor:1 | 1 (-1.43518) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.95866 HOMO: -7.28721 LUMO: -1.14016 factor:1 | 1 (-1.30100) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.24833 HOMO: -6.97156 LUMO: 0.51702 factor:1 | 1 (-0.59068) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87479 HOMO: -7.37156 LUMO: 0.29388 factor:1 | 1 (-1.21714) | 1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.67055 HOMO: -7.66273 LUMO: -1.59731 factor:1 | 1 (-0.01290) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.05802 HOMO: -7.50490 LUMO: -1.49935 factor:1 | 1 (-0.40036) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.87593 HOMO: -7.61102 LUMO: -1.45581 factor:1 | -1 (0.78173) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01156 HOMO: -7.58653 LUMO: -1.61091 factor:1 | 1 (-1.35390) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.65708 HOMO: -7.36068 LUMO: -1.14560 factor:1 | -1 (0.00057) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.84233 HOMO: -6.96339 LUMO: 0.26939 factor:1 | 1 (-1.18467) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.79991 HOMO: -6.53617 LUMO: 0.22313 factor:1 | 1 (-1.14225) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91145 HOMO: -7.33619 LUMO: -1.02587 factor:1 | 1 (-1.25379) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.07205 HOMO: -6.87904 LUMO: 0.33742 factor:1 | 1 (-1.41439) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.12973 HOMO: -6.88448 LUMO: 0.58777 factor:1 | -1 (0.52793) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.81083 HOMO: -6.55522 LUMO: -1.51295 factor:1 | 1 (-0.15317) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68695 HOMO: -7.43415 LUMO: 0.10612 factor:1 | 1 (-1.02930) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.43514 HOMO: -7.54300 LUMO: -0.02449 factor:1 | 1 (-0.77748) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68140 HOMO: -7.42054 LUMO: 0.28028 factor:1 | 1 (-1.02375) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.29108 HOMO: -6.98244 LUMO: -0.95784 factor:1 | 1 (-0.63343) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.90838 HOMO: -6.96884 LUMO: -1.12383 factor:1 | 1 (-0.25073) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.66348 HOMO: -6.80829 LUMO: -0.98233 factor:1 | 1 (-0.00582) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.84064 HOMO: -7.60830 LUMO: 0.58504 factor:1 | 1 (-1.18299) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80921 HOMO: -7.52123 LUMO: 0.08163 factor:1 | 1 (-1.15156) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.10993 HOMO: -7.59742 LUMO: 0.00272 factor:1 | 1 (-1.45227) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.86388 HOMO: -6.99333 LUMO: -1.33880 factor:1 | 1 (-1.20623) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.14634 HOMO: -6.63958 LUMO: -1.39322 factor:1 | 1 (-0.48869) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45576 HOMO: -7.86137 LUMO: 0.01633 factor:1 | 1 (-0.79811) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.52639 HOMO: -7.29537 LUMO: 0.14694 factor:1 | -1 (0.13127) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.61840 HOMO: -6.95523 LUMO: 0.48708 factor:1 | -1 (1.03926) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87890 HOMO: -7.10217 LUMO: -1.10478 factor:1 | 1 (-1.22125) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.86932 HOMO: -6.88176 LUMO: -0.96328 factor:1 | 1 (-1.21167) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64967 HOMO: -7.89130 LUMO: -0.13334 factor:1 | 1 (-0.99202) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59413 HOMO: -7.75252 LUMO: 0.25579 factor:1 | 1 (-0.93648) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60826 HOMO: -6.87632 LUMO: -0.93063 factor:1 | 1 (-0.95060) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.61672 HOMO: -6.78108 LUMO: -0.86804 factor:1 | 1 (-0.95907) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.78384 HOMO: -5.98106 LUMO: 0.10340 factor:1 | 1 (-2.12619) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.33698 HOMO: -6.40284 LUMO: -0.87349 factor:1 | 1 (-1.67932) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62967 HOMO: -6.77019 LUMO: -1.20819 factor:1 | 1 (-0.97202) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20190 HOMO: -6.90081 LUMO: -1.00682 factor:1 | 1 (-1.54425) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36838 HOMO: -6.59060 LUMO: -0.26667 factor:1 | 1 (-1.71073) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.57002 HOMO: -6.50896 LUMO: -0.48708 factor:1 | 1 (-1.91236) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.86293 HOMO: -6.20420 LUMO: -0.73471 factor:1 | 1 (-1.20527) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70861 HOMO: -6.17154 LUMO: -0.68573 factor:1 | 1 (-1.05096) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30277 HOMO: -6.21236 LUMO: 0.09796 factor:1 | 1 (-1.64512) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50645 HOMO: -6.38379 LUMO: 0.58232 factor:1 | 1 (-1.84880) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45898 HOMO: -7.42871 LUMO: 0.40273 factor:1 | 1 (-0.80132) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46330 HOMO: -6.54978 LUMO: 0.26395 factor:1 | 1 (-0.80565) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.35614 HOMO: -7.14027 LUMO: 0.14150 factor:1 | 1 (-1.69848) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.72251 HOMO: -7.25456 LUMO: -0.15783 factor:1 | 1 (-2.06485) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52050 HOMO: -6.90897 LUMO: 0.63403 factor:1 | 1 (-0.86285) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68597 HOMO: -6.49264 LUMO: 0.71022 factor:1 | 1 (-1.02832) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11665 HOMO: -6.56067 LUMO: -1.03947 factor:1 | 1 (-1.45899) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.71686 HOMO: -6.79196 LUMO: -1.12655 factor:1 | 1 (-1.05920) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70184 HOMO: -6.95251 LUMO: -1.09118 factor:1 | 1 (-1.04418) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.84173 HOMO: -7.47225 LUMO: -0.22041 factor:1 | 1 (-1.18408) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.77983 HOMO: -7.13483 LUMO: -0.98505 factor:1 | 1 (-0.12218) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.47857 HOMO: -6.99061 LUMO: -1.05852 factor:1 | 1 (-0.82091) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62608 HOMO: -6.52257 LUMO: -1.11022 factor:1 | 1 (-0.96843) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.39519 HOMO: -6.75114 LUMO: -1.09934 factor:1 | 1 (-0.73754) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77719 HOMO: -6.82189 LUMO: -0.89253 factor:1 | 1 (-1.11953) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.75977 HOMO: -6.83278 LUMO: -0.97961 factor:1 | 1 (-1.10212) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.40375 HOMO: -6.65318 LUMO: -0.84355 factor:1 | -1 (1.25390) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89444 HOMO: -6.75931 LUMO: -0.88437 factor:1 | 1 (-1.23678) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76758 HOMO: -6.19059 LUMO: -0.45715 factor:1 | 1 (-1.10993) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.66015 HOMO: -7.09673 LUMO: -2.01908 factor:1 | 1 (-1.00249) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45710 HOMO: -7.88042 LUMO: 0.38640 factor:1 | 1 (-0.79944) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.61768 HOMO: -7.83144 LUMO: 0.14422 factor:1 | -1 (0.03997) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.86847 HOMO: -7.46408 LUMO: 0.44627 factor:1 | 1 (-2.21082) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91063 HOMO: -7.12394 LUMO: -2.04902 factor:1 | 1 (-1.25298) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.12857 HOMO: -6.78380 LUMO: -1.11295 factor:1 | 1 (-1.47091) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46262 HOMO: -7.12938 LUMO: -0.23674 factor:1 | 1 (-0.80497) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77700 HOMO: -6.14705 LUMO: -0.20409 factor:1 | 1 (-1.11934) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.92074 HOMO: -6.50080 LUMO: -0.28300 factor:1 | 1 (-2.26309) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.90108 HOMO: -6.50352 LUMO: -0.62042 factor:1 | 1 (-1.24342) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.85448 HOMO: -6.46543 LUMO: -0.53879 factor:1 | 1 (-2.19683) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17564 HOMO: -7.32803 LUMO: -0.52790 factor:1 | 1 (-1.51799) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50864 HOMO: -5.94025 LUMO: -0.17687 factor:1 | 1 (-0.85098) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.28571 HOMO: -5.62187 LUMO: 0.05714 factor:1 | 1 (-1.62806) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80864 HOMO: -7.03414 LUMO: -1.04492 factor:1 | 1 (-1.15099) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62970 HOMO: -6.75387 LUMO: -2.02181 factor:1 | 1 (-0.97205) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.36270 HOMO: -6.55250 LUMO: -0.75648 factor:1 | 1 (-0.70505) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.38619 HOMO: -6.81101 LUMO: -1.02043 factor:1 | 1 (-0.72853) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89670 HOMO: -6.69672 LUMO: -2.81910 factor:1 | 1 (-1.23904) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.36447 HOMO: -6.69128 LUMO: -2.58236 factor:1 | 1 (-0.70682) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.15551 HOMO: -6.73482 LUMO: -2.06807 factor:1 | 1 (-1.49785) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.43410 HOMO: -7.66545 LUMO: 0.17143 factor:1 | 1 (-0.77645) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.75460 HOMO: -6.87904 LUMO: -1.25172 factor:1 | 1 (-1.09695) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.09850 HOMO: -6.84366 LUMO: -0.19320 factor:1 | 1 (-1.44084) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.34879 HOMO: -6.97972 LUMO: -0.97961 factor:1 | 1 (-1.69113) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52140 HOMO: -6.72121 LUMO: -0.70477 factor:1 | 1 (-0.86374) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.36531 HOMO: -7.18925 LUMO: 0.40001 factor:1 | 1 (-0.70766) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.42842 HOMO: -6.72121 LUMO: 0.19592 factor:1 | 1 (-0.77076) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.52971 HOMO: -6.85999 LUMO: -0.39457 factor:1 | -1 (0.12795) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36887 HOMO: -6.90625 LUMO: 0.05987 factor:1 | 1 (-1.71122) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64121 HOMO: -7.00421 LUMO: 0.37552 factor:1 | 1 (-0.98356) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20963 HOMO: -6.56883 LUMO: -0.97689 factor:1 | 1 (-1.55197) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27998 HOMO: -6.66679 LUMO: 0.56055 factor:1 | 1 (-0.62232) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91847 HOMO: -6.75931 LUMO: 0.32926 factor:1 | 1 (-1.26081) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.77797 HOMO: -6.53617 LUMO: -1.06397 factor:1 | 1 (-2.12031) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.40737 HOMO: -6.78108 LUMO: 0.42722 factor:1 | 1 (-2.74971) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.15749 HOMO: -7.05319 LUMO: 0.61498 factor:1 | 1 (-1.49984) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.62558 HOMO: -6.78380 LUMO: 1.49391 factor:1 | 1 (-1.96793) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.41448 HOMO: -7.21102 LUMO: 0.27211 factor:1 | 1 (-1.75682) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.48097 HOMO: -6.67223 LUMO: 0.81362 factor:1 | 1 (-2.82332) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.84379 HOMO: -6.69944 LUMO: 1.40683 factor:1 | 1 (-2.18614) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.48689 HOMO: -7.02598 LUMO: 1.46941 factor:1 | 1 (-1.82923) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.99975 HOMO: -5.85045 LUMO: -0.76736 factor:1 | 1 (-1.34209) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46333 HOMO: -6.53890 LUMO: -0.50885 factor:1 | 1 (-0.80567) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.91280 HOMO: -6.42733 LUMO: -0.63947 factor:1 | 1 (-2.25514) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11510 HOMO: -6.82189 LUMO: -0.85444 factor:1 | 1 (-1.45744) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.63297 HOMO: -6.97428 LUMO: -1.22179 factor:1 | 1 (-2.97532) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.93868 HOMO: -6.93346 LUMO: -1.09934 factor:1 | 1 (-2.28102) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.52000 HOMO: -7.17292 LUMO: -1.11839 factor:1 | 1 (-1.86235) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.72120 HOMO: -7.00965 LUMO: -1.23268 factor:1 | 1 (-2.06355) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.18657 HOMO: -6.73210 LUMO: -1.12383 factor:1 | 1 (-2.52892) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.55840 HOMO: -7.61375 LUMO: -0.11973 factor:1 | 1 (-1.90074) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.79132 HOMO: -7.42327 LUMO: 0.41906 factor:1 | 1 (-3.13366) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.84552 HOMO: -6.94162 LUMO: -1.01771 factor:1 | 1 (-3.18787) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.38163 HOMO: -6.82189 LUMO: -0.92791 factor:1 | 1 (-1.72398) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.66313 HOMO: -6.92258 LUMO: -1.73881 factor:1 | 1 (-2.00548) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.94981 HOMO: -6.50896 LUMO: -1.60819 factor:1 | 1 (-2.29215) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.21796 HOMO: -6.38379 LUMO: -2.18780 factor:1 | 1 (-1.56030) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.03471 HOMO: -6.48992 LUMO: -0.97417 factor:1 | 1 (-2.37705) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36177 HOMO: -6.01644 LUMO: -0.04354 factor:1 | 1 (-1.70411) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.97749 HOMO: -6.70761 LUMO: -0.14422 factor:1 | 1 (-1.31983) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.08554 HOMO: -6.70216 LUMO: 0.14422 factor:1 | 1 (-2.42788) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.09860 HOMO: -7.07224 LUMO: -0.10885 factor:1 | 1 (-2.44094) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.44950 HOMO: -7.52667 LUMO: -0.74287 factor:1 | 1 (-1.79184) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01771 HOMO: -6.48447 LUMO: -0.96056 factor:1 | 1 (-1.36005) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.48778 HOMO: -6.22597 LUMO: -0.41361 factor:1 | 1 (-2.83012) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.41771 HOMO: -6.12256 LUMO: -1.05852 factor:1 | 1 (-1.76006) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.12744 HOMO: -6.97428 LUMO: -0.60681 factor:1 | 1 (-2.46979) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.29902 HOMO: -6.78380 LUMO: -0.88981 factor:1 | 1 (-1.64136) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.32243 HOMO: -6.85999 LUMO: 0.07891 factor:1 | 1 (-0.66477) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36653 HOMO: -7.08312 LUMO: -0.60137 factor:1 | 1 (-1.70888) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.23562 HOMO: -6.57699 LUMO: -0.68028 factor:1 | 1 (-0.57797) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30226 HOMO: -6.09807 LUMO: -0.31837 factor:1 | 1 (-1.64460) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68350 HOMO: -6.10624 LUMO: 0.14966 factor:1 | 1 (-1.02584) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.73081 HOMO: -6.77019 LUMO: -0.95784 factor:1 | 1 (-2.07315) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64360 HOMO: -5.93208 LUMO: -0.44627 factor:1 | 1 (-0.98595) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.55361 HOMO: -6.12256 LUMO: -0.27756 factor:1 | 1 (-1.89595) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.29576 HOMO: -5.98106 LUMO: -0.37824 factor:1 | 1 (-0.63811) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57313 HOMO: -7.06408 LUMO: -1.12927 factor:1 | 1 (-0.91547) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20402 HOMO: -6.70761 LUMO: -0.98505 factor:1 | 1 (-1.54637) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27168 HOMO: -7.00965 LUMO: -0.42722 factor:1 | 1 (-0.61402) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.41332 HOMO: -5.96201 LUMO: -0.59049 factor:1 | 1 (-0.75566) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.96192 HOMO: -6.34570 LUMO: -1.68438 factor:1 | 1 (-2.30426) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61946 HOMO: -6.97156 LUMO: -1.85854 factor:1 | 1 (-1.96180) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50501 HOMO: -5.91848 LUMO: -2.51433 factor:1 | 1 (-1.84735) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.71266 HOMO: -6.39195 LUMO: -1.66262 factor:1 | 1 (-2.05500) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20000 HOMO: -6.50352 LUMO: 0.19592 factor:1 | 1 (-1.54234) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.15173 HOMO: -6.45998 LUMO: 0.34831 factor:1 | 1 (-0.49408) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.38362 HOMO: -7.05319 LUMO: 0.23402 factor:1 | 1 (-1.72596) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.41356 HOMO: -6.61237 LUMO: 0.18232 factor:1 | 1 (-0.75591) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17902 HOMO: -6.57427 LUMO: 0.40545 factor:1 | 1 (-1.52136) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.55212 HOMO: -7.26544 LUMO: 0.41089 factor:1 | 1 (-0.89447) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64679 HOMO: -6.26406 LUMO: -0.85444 factor:1 | 1 (-0.98913) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.97625 HOMO: -6.25318 LUMO: -0.79457 factor:1 | 1 (-0.31859) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.78108 HOMO: -6.68040 LUMO: 0.41089 factor:1 | 1 (-1.12342) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.83139 HOMO: -6.37835 LUMO: 0.37280 factor:1 | 1 (-1.17374) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.18915 HOMO: -6.56067 LUMO: 0.62858 factor:1 | 1 (-0.53149) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68897 HOMO: -6.74026 LUMO: -0.04082 factor:1 | 1 (-1.03131) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.48445 HOMO: -6.53617 LUMO: 0.35103 factor:1 | 1 (-0.82679) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.82630 HOMO: -6.51985 LUMO: 0.25851 factor:1 | 1 (-1.16865) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85049 HOMO: -6.58788 LUMO: -1.98371 factor:1 | 1 (-1.19284) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60619 HOMO: -6.51441 LUMO: 0.29116 factor:1 | 1 (-0.94853) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.96493 HOMO: -6.81101 LUMO: 0.35647 factor:1 | 1 (-0.30727) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64513 HOMO: -6.42733 LUMO: 0.10340 factor:1 | 1 (-0.98747) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91517 HOMO: -6.70761 LUMO: 0.28028 factor:1 | 1 (-1.25752) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77659 HOMO: -6.67495 LUMO: 0.01633 factor:1 | 1 (-1.11893) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.22588 HOMO: -6.75387 LUMO: 0.15510 factor:1 | 1 (-0.56823) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76018 HOMO: -6.56067 LUMO: 0.35919 factor:1 | 1 (-1.10252) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69691 HOMO: -7.16748 LUMO: 0.21497 factor:1 | 1 (-1.03926) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50779 HOMO: -6.71849 LUMO: 0.26667 factor:1 | 1 (-0.85014) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.78617 HOMO: -6.69128 LUMO: 0.55783 factor:1 | 1 (-1.12851) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85038 HOMO: -6.71305 LUMO: 0.45987 factor:1 | 1 (-1.19273) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.10897 HOMO: -5.90487 LUMO: -0.70750 factor:1 | 1 (-2.45131) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23409 HOMO: -6.84638 LUMO: -0.72110 factor:1 | 1 (-1.57644) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.62047 HOMO: -6.66135 LUMO: -1.13471 factor:1 | 1 (-1.96281) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.74325 HOMO: -6.74026 LUMO: -0.64763 factor:1 | 1 (-1.08560) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.66594 HOMO: -6.69672 LUMO: -1.05036 factor:1 | 1 (-2.00828) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57038 HOMO: -6.78924 LUMO: -1.03675 factor:1 | 1 (-0.91272) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.90790 HOMO: -6.81373 LUMO: -0.85988 factor:1 | 1 (-2.25025) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01553 HOMO: -7.26544 LUMO: 0.91158 factor:1 | 1 (-1.35788) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.80085 HOMO: -6.64230 LUMO: -1.92929 factor:1 | 1 (-2.14320) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80086 HOMO: -7.20830 LUMO: 0.11429 factor:1 | 1 (-1.14320) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50333 HOMO: -7.17020 LUMO: 0.04898 factor:1 | 1 (-0.84568) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.71781 HOMO: -7.16476 LUMO: 0.04898 factor:1 | 1 (-1.06016) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.78820 HOMO: -6.59332 LUMO: -0.49253 factor:1 | 1 (-2.13054) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.29681 HOMO: -7.46953 LUMO: 0.84083 factor:1 | 1 (-1.63916) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50899 HOMO: -7.39878 LUMO: 0.88709 factor:1 | 1 (-0.85134) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.03004 HOMO: -6.84094 LUMO: -0.61498 factor:1 | 1 (-0.37239) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59835 HOMO: -6.03549 LUMO: -0.27211 factor:1 | 1 (-0.94070) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.52210 HOMO: -7.31170 LUMO: -0.64763 factor:1 | 1 (-1.86444) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.37761 HOMO: -6.88992 LUMO: -0.84627 factor:1 | 1 (-0.71996) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.96747 HOMO: -7.12666 LUMO: -0.09252 factor:1 | 1 (-2.30981) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.56051 HOMO: -6.70489 LUMO: -0.63675 factor:1 | 1 (-2.90286) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.41821 HOMO: -6.98788 LUMO: 0.86804 factor:1 | 1 (-0.76056) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.71622 HOMO: -6.80285 LUMO: -0.60954 factor:1 | 1 (-2.05857) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.48064 HOMO: -7.02054 LUMO: -0.74287 factor:1 | -1 (0.17701) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.72281 HOMO: -7.03686 LUMO: -0.81090 factor:1 | 1 (-2.06515) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.93552 HOMO: -6.70489 LUMO: -1.00954 factor:1 | 1 (-2.27787) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64282 HOMO: -7.69810 LUMO: 0.00544 factor:1 | 1 (-0.98516) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60178 HOMO: -6.83550 LUMO: -0.11157 factor:1 | 1 (-0.94413) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62126 HOMO: -6.76203 LUMO: -2.13609 factor:1 | 1 (-0.96361) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.51776 HOMO: -6.72121 LUMO: -2.62862 factor:1 | 1 (-2.86011) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61864 HOMO: -6.48719 LUMO: -2.73474 factor:1 | 1 (-1.96099) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.21066 HOMO: -6.83006 LUMO: -0.00544 factor:1 | 1 (-1.55301) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.67475 HOMO: -6.84094 LUMO: -1.11022 factor:1 | 1 (-2.01710) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.24073 HOMO: -6.66951 LUMO: -1.23812 factor:1 | 1 (-1.58308) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.85606 HOMO: -6.78380 LUMO: -1.27894 factor:1 | 1 (-2.19841) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.44547 HOMO: -6.50352 LUMO: -0.56055 factor:1 | 1 (-1.78782) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.64594 HOMO: -7.77974 LUMO: -0.26395 factor:1 | 1 (-1.98828) | 1 | 1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.26122 HOMO: -7.01510 LUMO: -1.64085 factor:1 | 1 (-1.60357) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.43488 HOMO: -6.59876 LUMO: -0.91158 factor:1 | 1 (-1.77723) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45326 HOMO: -4.67219 LUMO: -0.67756 factor:1 | 1 (-0.79561) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27641 HOMO: -6.70489 LUMO: -0.65579 factor:1 | 1 (-0.61876) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70116 HOMO: -6.62325 LUMO: -0.60409 factor:1 | 1 (-1.04350) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59963 HOMO: -6.20147 LUMO: 0.15238 factor:1 | 1 (-0.94198) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59068 HOMO: -6.43549 LUMO: -0.07075 factor:1 | 1 (-0.93302) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.92835 HOMO: -7.02054 LUMO: 0.13061 factor:1 | 1 (-0.27070) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.65019 HOMO: -7.04503 LUMO: 0.30749 factor:1 | 1 (-0.99254) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89858 HOMO: -6.74842 LUMO: -0.99594 factor:1 | 1 (-1.24092) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.44415 HOMO: -6.35658 LUMO: 0.41633 factor:1 | 1 (-0.78649) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.33788 HOMO: -6.79740 LUMO: 0.56872 factor:1 | 1 (-1.68022) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.51021 HOMO: -6.51713 LUMO: -0.05987 factor:1 | 1 (-0.85256) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.22642 HOMO: -6.68040 LUMO: 0.34558 factor:1 | 1 (-1.56876) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.72404 HOMO: -6.39740 LUMO: 0.50069 factor:1 | 1 (-1.06639) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50015 HOMO: -6.91713 LUMO: -0.97145 factor:1 | 1 (-0.84249) | -1 | -1 |
| G: -6694.29196 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.26107 HOMO: -7.10761 LUMO: -0.27483 factor:1 | 1 (-0.60341) | 1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.63887 HOMO: -6.98788 LUMO: 0.40273 factor:1 | 1 (-0.72102) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.02017 HOMO: -6.87087 LUMO: 0.28572 factor:1 | -1 (0.89768) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.96118 HOMO: -7.36612 LUMO: -0.12245 factor:1 | -1 (0.95667) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.84865 HOMO: -6.72938 LUMO: 0.33742 factor:1 | -1 (0.06920) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.03949 HOMO: -7.32531 LUMO: 0.07619 factor:1 | 1 (-0.12163) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60491 HOMO: -6.87087 LUMO: -0.08436 factor:1 | 1 (-0.68706) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.94545 HOMO: -6.67495 LUMO: 0.85988 factor:1 | -1 (0.97240) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.22447 HOMO: -6.96339 LUMO: 0.65307 factor:1 | 1 (-0.30662) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.35449 HOMO: -6.58516 LUMO: -0.78641 factor:1 | -1 (0.56336) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.47621 HOMO: -6.56883 LUMO: 0.44355 factor:1 | -1 (0.44164) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.99465 HOMO: -6.68312 LUMO: 0.43538 factor:1 | -1 (0.92320) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.57031 HOMO: -6.81917 LUMO: 0.20681 factor:1 | -1 (0.34754) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.71790 HOMO: -6.91169 LUMO: 0.08163 factor:1 | -1 (0.19995) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.33816 HOMO: -4.88444 LUMO: -0.49253 factor:1 | 1 (-0.42031) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.89367 HOMO: -6.42189 LUMO: 0.64763 factor:1 | -1 (1.02418) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.38072 HOMO: -6.24501 LUMO: 0.55783 factor:1 | -1 (0.53713) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.69654 HOMO: -6.41372 LUMO: 0.29388 factor:1 | -1 (0.22131) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.62337 HOMO: -5.67902 LUMO: 1.77690 factor:1 | -1 (0.29448) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.14289 HOMO: -6.55794 LUMO: 0.05170 factor:1 | 1 (-0.22504) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.51496 HOMO: -6.52801 LUMO: 0.25851 factor:1 | -1 (0.40289) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.77865 HOMO: -7.08857 LUMO: 0.11157 factor:1 | -1 (1.13920) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.98790 HOMO: -6.58243 LUMO: 0.75648 factor:1 | -1 (0.92995) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.61189 HOMO: -7.22190 LUMO: 0.45171 factor:1 | -1 (0.30596) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.86825 HOMO: -6.47087 LUMO: 0.00000 factor:1 | -1 (1.04960) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.98287 HOMO: -6.78652 LUMO: 1.32247 factor:1 | -1 (0.93498) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.49322 HOMO: -6.74026 LUMO: 1.45309 factor:1 | -1 (0.42463) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.48845 HOMO: -6.69944 LUMO: 0.76464 factor:1 | -1 (0.42940) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.41879 HOMO: -6.62325 LUMO: 0.64763 factor:1 | -1 (0.49906) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.49959 HOMO: -6.45182 LUMO: 0.49253 factor:1 | -1 (1.41826) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.58626 HOMO: -7.14843 LUMO: 0.62586 factor:1 | -1 (1.33159) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.73620 HOMO: -6.87087 LUMO: 1.53200 factor:1 | -1 (1.18165) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.77799 HOMO: -6.54978 LUMO: 0.45171 factor:1 | -1 (1.13986) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.43230 HOMO: -6.63686 LUMO: 0.80001 factor:1 | -1 (1.48555) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.84327 HOMO: -7.00693 LUMO: 1.56193 factor:1 | -1 (1.07458) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.37588 HOMO: -6.02460 LUMO: 1.72792 factor:1 | -1 (0.54197) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.43419 HOMO: -6.36746 LUMO: -1.20002 factor:1 | -1 (0.48366) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.51915 HOMO: -7.26816 LUMO: -1.06397 factor:1 | -1 (0.39870) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.23035 HOMO: -7.34707 LUMO: -1.09662 factor:1 | -1 (0.68750) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.81380 HOMO: -7.93212 LUMO: -0.13606 factor:1 | -1 (1.10405) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.45841 HOMO: -6.80285 LUMO: 0.58504 factor:1 | -1 (0.45944) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.69975 HOMO: -7.12938 LUMO: 0.32926 factor:1 | -1 (0.21810) | 1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.45477 HOMO: -6.86815 LUMO: -1.30070 factor:1 | -1 (0.46308) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.60867 HOMO: -6.99333 LUMO: -1.03947 factor:1 | -1 (0.30918) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.27404 HOMO: -7.56749 LUMO: -0.11157 factor:1 | -1 (1.64381) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.54278 HOMO: -7.57293 LUMO: -0.07891 factor:1 | -1 (1.37507) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.69641 HOMO: -7.30626 LUMO: 0.27211 factor:1 | -1 (1.22144) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.84360 HOMO: -7.77974 LUMO: 0.27211 factor:1 | -1 (1.07425) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.70558 HOMO: -7.11578 LUMO: 0.19864 factor:1 | -1 (1.21227) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.40652 HOMO: -7.71171 LUMO: 0.57688 factor:1 | -1 (0.51133) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.87470 HOMO: -7.83688 LUMO: 0.37824 factor:1 | -1 (1.04315) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.00730 HOMO: -6.94979 LUMO: -1.66534 factor:1 | -1 (0.91055) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.38837 HOMO: -6.97156 LUMO: -1.13199 factor:1 | -1 (0.52948) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.34170 HOMO: -6.91441 LUMO: -1.08301 factor:1 | -1 (0.57615) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.42769 HOMO: -6.71849 LUMO: -0.74831 factor:1 | -1 (0.49016) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.60675 HOMO: -7.09401 LUMO: -1.77690 factor:1 | -1 (1.31110) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.81437 HOMO: -6.97156 LUMO: -1.45037 factor:1 | -1 (1.10348) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.77655 HOMO: -7.22462 LUMO: -1.11295 factor:1 | -1 (1.14130) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.05734 HOMO: -7.85321 LUMO: 0.16599 factor:1 | 1 (-0.13949) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.11902 HOMO: -7.71987 LUMO: 0.55511 factor:1 | 1 (-0.20117) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57136 HOMO: -7.63551 LUMO: 0.14422 factor:1 | 1 (-0.65351) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.43413 HOMO: -6.98788 LUMO: -0.80546 factor:1 | 1 (-0.51628) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70157 HOMO: -6.98788 LUMO: -1.16737 factor:1 | 1 (-0.78372) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.90530 HOMO: -6.56611 LUMO: -1.60819 factor:1 | 1 (-0.98745) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61590 HOMO: -6.95251 LUMO: 0.66396 factor:1 | 1 (-1.69804) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.32256 HOMO: -7.35252 LUMO: 0.49797 factor:1 | 1 (-1.40471) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.32286 HOMO: -6.90897 LUMO: -0.81090 factor:1 | 1 (-0.40501) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.32844 HOMO: -7.04503 LUMO: -1.08301 factor:1 | 1 (-0.41059) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14242 HOMO: -6.92530 LUMO: -1.29526 factor:1 | 1 (-1.22457) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.99322 HOMO: -6.93074 LUMO: -1.25444 factor:1 | 1 (-1.07537) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.22207 HOMO: -6.73482 LUMO: -0.62042 factor:1 | 1 (-0.30422) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.33846 HOMO: -7.67633 LUMO: 0.59593 factor:1 | 1 (-0.42061) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.19110 HOMO: -7.39061 LUMO: -0.19320 factor:1 | 1 (-1.27325) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17722 HOMO: -7.55388 LUMO: -0.20136 factor:1 | 1 (-1.25937) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.02557 HOMO: -7.14027 LUMO: -0.99866 factor:1 | 1 (-1.10772) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.26425 HOMO: -6.75931 LUMO: -0.73199 factor:1 | 1 (-0.34640) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.19676 HOMO: -5.45044 LUMO: -0.18776 factor:1 | 1 (-1.27891) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.94447 HOMO: -6.70761 LUMO: -0.84083 factor:1 | 1 (-2.02662) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.17552 HOMO: -6.05453 LUMO: -1.06669 factor:1 | 1 (-2.25767) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.06907 HOMO: -6.86815 LUMO: -0.98233 factor:1 | 1 (-2.15122) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.90021 HOMO: -6.73210 LUMO: -0.95240 factor:1 | 1 (-0.98236) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01561 HOMO: -5.89671 LUMO: -1.05036 factor:1 | 1 (-1.09776) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.39316 HOMO: -7.61102 LUMO: 0.33470 factor:1 | 1 (-2.47531) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.05207 HOMO: -7.51034 LUMO: 0.23674 factor:1 | 1 (-2.13422) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.34079 HOMO: -7.41510 LUMO: 0.62858 factor:1 | 1 (-1.42294) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.32166 HOMO: -6.76203 LUMO: -1.72792 factor:1 | 1 (-1.40381) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.29031 HOMO: -6.60420 LUMO: -0.45715 factor:1 | 1 (-1.37246) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.64528 HOMO: -6.59060 LUMO: -0.58232 factor:1 | 1 (-1.72743) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.64387 HOMO: -7.43687 LUMO: -0.76736 factor:1 | 1 (-1.72602) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.63356 HOMO: -6.08719 LUMO: -0.48708 factor:1 | 1 (-1.71571) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.56169 HOMO: -5.88854 LUMO: -0.05714 factor:1 | 1 (-1.64384) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.75075 HOMO: -7.34435 LUMO: -0.71838 factor:1 | 1 (-1.83290) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.72543 HOMO: -7.46408 LUMO: -0.63130 factor:1 | 1 (-0.80758) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.08680 HOMO: -7.00965 LUMO: -1.24900 factor:1 | 1 (-1.16895) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.07806 HOMO: -6.91169 LUMO: -0.88981 factor:1 | 1 (-1.16021) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61802 HOMO: -6.78652 LUMO: -0.82178 factor:1 | 1 (-1.70017) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.39189 HOMO: -7.80423 LUMO: 0.87076 factor:1 | 1 (-1.47404) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.46705 HOMO: -6.97700 LUMO: -1.00954 factor:1 | 1 (-1.54920) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50338 HOMO: -6.92530 LUMO: -0.88165 factor:1 | 1 (-1.58553) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.37259 HOMO: -7.14571 LUMO: -1.04492 factor:1 | -1 (0.54526) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.34846 HOMO: -7.49674 LUMO: 0.34558 factor:1 | 1 (-1.43061) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.27950 HOMO: -6.44094 LUMO: -1.20819 factor:1 | 1 (-2.36165) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.08262 HOMO: -6.47359 LUMO: -1.14016 factor:1 | 1 (-2.16477) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30188 HOMO: -6.61237 LUMO: -0.87076 factor:1 | 1 (-1.38403) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.99265 HOMO: -6.73754 LUMO: -1.09662 factor:1 | 1 (-1.07480) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85828 HOMO: -6.97700 LUMO: 0.13061 factor:1 | 1 (-0.94043) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.70827 HOMO: -6.82734 LUMO: 0.59865 factor:1 | -1 (0.20958) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.33518 HOMO: -6.86543 LUMO: -0.91430 factor:1 | 1 (-1.41733) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.51894 HOMO: -6.74298 LUMO: 0.28028 factor:1 | 1 (-1.60109) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.62153 HOMO: -6.75387 LUMO: 0.19592 factor:1 | 1 (-1.70368) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.23651 HOMO: -7.05591 LUMO: 0.10612 factor:1 | 1 (-2.31865) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.95772 HOMO: -6.86543 LUMO: 0.49253 factor:1 | 1 (-2.03987) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.34931 HOMO: -6.11440 LUMO: -1.12655 factor:1 | 1 (-1.43145) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36041 HOMO: -6.77291 LUMO: -1.02859 factor:1 | 1 (-1.44256) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46777 HOMO: -6.54978 LUMO: 0.29116 factor:1 | 1 (-0.54991) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.24041 HOMO: -7.18108 LUMO: 0.00000 factor:1 | 1 (-1.32255) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14253 HOMO: -6.86271 LUMO: -1.15376 factor:1 | 1 (-1.22468) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50823 HOMO: -6.78108 LUMO: -1.22723 factor:1 | 1 (-0.59038) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.40899 HOMO: -6.40828 LUMO: 0.02449 factor:1 | 1 (-0.49114) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.57270 HOMO: -6.43821 LUMO: 0.09796 factor:1 | 1 (-2.65485) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.97362 HOMO: -6.99877 LUMO: 0.40545 factor:1 | 1 (-2.05577) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.83024 HOMO: -6.68856 LUMO: 0.19320 factor:1 | 1 (-1.91239) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.81624 HOMO: -7.11034 LUMO: 0.31293 factor:1 | 1 (-2.89839) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.40586 HOMO: -6.92530 LUMO: -0.85444 factor:1 | 1 (-0.48801) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20250 HOMO: -6.60148 LUMO: -0.59865 factor:1 | 1 (-1.28465) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60290 HOMO: -6.72938 LUMO: 0.30749 factor:1 | 1 (-0.68505) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.39741 HOMO: -7.31170 LUMO: 0.06803 factor:1 | 1 (-1.47956) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.28195 HOMO: -7.09129 LUMO: -0.04626 factor:1 | 1 (-2.36410) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.46345 HOMO: -6.38379 LUMO: -0.76736 factor:1 | 1 (-2.54560) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.54953 HOMO: -6.13617 LUMO: -0.63947 factor:1 | 1 (-1.63168) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.28562 HOMO: -6.92258 LUMO: 0.37007 factor:1 | 1 (-2.36777) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.60164 HOMO: -6.35930 LUMO: 0.41361 factor:1 | 1 (-1.68379) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.41758 HOMO: -6.60420 LUMO: 0.26667 factor:1 | 1 (-1.49973) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.19841 HOMO: -6.04909 LUMO: 1.82588 factor:1 | 1 (-2.28056) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.83965 HOMO: -6.69672 LUMO: 1.72520 factor:1 | 1 (-1.92180) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.54482 HOMO: -6.50080 LUMO: 0.29116 factor:1 | 1 (-1.62697) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.94965 HOMO: -6.60692 LUMO: -0.43266 factor:1 | 1 (-1.03180) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.93248 HOMO: -6.93890 LUMO: 0.39729 factor:1 | 1 (-1.01463) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.04886 HOMO: -6.52801 LUMO: -0.47076 factor:1 | 1 (-1.13101) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05474 HOMO: -6.41100 LUMO: 0.30477 factor:1 | 1 (-1.13689) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.93931 HOMO: -6.37291 LUMO: -0.80001 factor:1 | 1 (-1.02146) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.19093 HOMO: -6.51985 LUMO: 1.44765 factor:1 | 1 (-2.27308) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.51129 HOMO: -6.64774 LUMO: 0.04626 factor:1 | 1 (-1.59344) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.51423 HOMO: -6.65863 LUMO: 0.29933 factor:1 | 1 (-1.59638) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69974 HOMO: -7.09673 LUMO: 0.28300 factor:1 | 1 (-0.78189) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.04418 HOMO: -6.57155 LUMO: -1.11567 factor:1 | 1 (-2.12632) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30291 HOMO: -6.38379 LUMO: -0.60681 factor:1 | 1 (-1.38506) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.92093 HOMO: -6.60148 LUMO: 0.18232 factor:1 | 1 (-2.00308) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.20886 HOMO: -6.96067 LUMO: -0.52246 factor:1 | 1 (-2.29101) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.36843 HOMO: -6.57427 LUMO: -0.84627 factor:1 | 1 (-2.45058) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.76123 HOMO: -6.59332 LUMO: -0.98233 factor:1 | 1 (-1.84338) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87215 HOMO: -6.20692 LUMO: -0.27483 factor:1 | 1 (-0.95430) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.87800 HOMO: -6.81373 LUMO: 0.74559 factor:1 | 1 (-1.96014) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.79724 HOMO: -6.60420 LUMO: 0.54695 factor:1 | 1 (-0.87939) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.73715 HOMO: -6.58788 LUMO: -0.31021 factor:1 | 1 (-1.81930) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.76556 HOMO: -6.72938 LUMO: 0.64763 factor:1 | 1 (-1.84771) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.84975 HOMO: -6.86815 LUMO: 0.32109 factor:1 | 1 (-1.93190) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69588 HOMO: -6.63141 LUMO: 0.18776 factor:1 | 1 (-0.77803) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.76787 HOMO: -7.18653 LUMO: 0.09524 factor:1 | 1 (-1.85002) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.51984 HOMO: -6.83550 LUMO: 0.03537 factor:1 | 1 (-1.60199) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.53419 HOMO: -7.47769 LUMO: 0.40817 factor:1 | 1 (-0.61634) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.00905 HOMO: -6.57971 LUMO: -0.63675 factor:1 | 1 (-1.09120) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.00541 HOMO: -6.74842 LUMO: -0.16327 factor:1 | 1 (-1.08756) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.38572 HOMO: -7.07224 LUMO: 0.61770 factor:1 | 1 (-0.46787) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.14954 HOMO: -6.83006 LUMO: 0.54695 factor:1 | -1 (0.76831) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.02753 HOMO: -6.60148 LUMO: 1.23540 factor:1 | 1 (-1.10968) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88380 HOMO: -6.99061 LUMO: 0.41089 factor:1 | 1 (-0.96595) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.32526 HOMO: -6.63686 LUMO: 0.85172 factor:1 | 1 (-0.40741) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01548 HOMO: -6.50624 LUMO: 0.12517 factor:1 | 1 (-1.09763) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.78048 HOMO: -6.35658 LUMO: 0.36463 factor:1 | 1 (-0.86263) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76238 HOMO: -6.34570 LUMO: 0.65035 factor:1 | 1 (-0.84453) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.13011 HOMO: -6.63141 LUMO: 1.25717 factor:1 | 1 (-2.21226) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.24772 HOMO: -6.91441 LUMO: 1.32792 factor:1 | 1 (-1.32987) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.04143 HOMO: -7.15387 LUMO: 0.64219 factor:1 | 1 (-2.12358) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.98486 HOMO: -7.17836 LUMO: 0.60409 factor:1 | 1 (-1.06701) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91267 HOMO: -6.92258 LUMO: 0.49525 factor:1 | 1 (-0.99482) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.68166 HOMO: -6.31032 LUMO: 0.48708 factor:1 | 1 (-2.76381) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.12992 HOMO: -6.49808 LUMO: 0.31021 factor:1 | 1 (-2.21207) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.64881 HOMO: -6.48447 LUMO: 0.37552 factor:1 | 1 (-2.73096) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.10682 HOMO: -6.66135 LUMO: -1.08301 factor:1 | 1 (-2.18897) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.58945 HOMO: -6.33481 LUMO: -0.51974 factor:1 | 1 (-1.67160) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.58980 HOMO: -6.76475 LUMO: -0.15238 factor:1 | 1 (-1.67195) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.08772 HOMO: -6.93346 LUMO: -0.10885 factor:1 | 1 (-1.16987) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.69851 HOMO: -7.19741 LUMO: 0.73199 factor:1 | 1 (-1.78066) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.86062 HOMO: -6.82734 LUMO: 0.88437 factor:1 | 1 (-0.94277) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.84051 HOMO: -7.01237 LUMO: 0.02721 factor:1 | 1 (-0.92266) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.09793 HOMO: -6.39195 LUMO: 1.46941 factor:1 | 1 (-1.18008) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.97599 HOMO: -6.53890 LUMO: 1.32792 factor:1 | 1 (-1.05814) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89485 HOMO: -6.82734 LUMO: 1.98099 factor:1 | 1 (-0.97700) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06778 HOMO: -6.74570 LUMO: 1.68983 factor:1 | 1 (-1.14993) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01877 HOMO: -6.41100 LUMO: 1.39050 factor:1 | 1 (-1.10092) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76984 HOMO: -5.92664 LUMO: 1.65989 factor:1 | 1 (-0.85199) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.92092 HOMO: -6.07630 LUMO: 1.54833 factor:1 | 1 (-1.00307) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.63718 HOMO: -6.45998 LUMO: 0.68573 factor:1 | 1 (-0.71933) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77204 HOMO: -6.52801 LUMO: 0.41361 factor:1 | 1 (-0.85419) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.35545 HOMO: -6.77564 LUMO: 0.42178 factor:1 | -1 (0.56240) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.85269 HOMO: -6.56339 LUMO: 1.65717 factor:1 | 1 (-1.93484) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.87609 HOMO: -5.85861 LUMO: 1.90752 factor:1 | 1 (-1.95824) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.77575 HOMO: -6.77019 LUMO: -2.48440 factor:1 | -1 (0.14210) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.20256 HOMO: -6.53890 LUMO: -1.82588 factor:1 | 1 (-0.28471) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.25694 HOMO: -6.50352 LUMO: -1.66806 factor:1 | 1 (-2.33909) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.35542 HOMO: -6.90625 LUMO: 0.43538 factor:1 | 1 (-2.43757) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.85875 HOMO: -6.85455 LUMO: 0.53062 factor:1 | 1 (-2.94090) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.56982 HOMO: -6.49536 LUMO: 0.31021 factor:1 | 1 (-2.65197) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.27461 HOMO: -4.97696 LUMO: -0.09252 factor:1 | 1 (-1.35676) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88415 HOMO: -5.31166 LUMO: 0.34286 factor:1 | 1 (-0.96630) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.83476 HOMO: -6.42461 LUMO: 0.74287 factor:1 | 1 (-0.91691) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.31880 HOMO: -6.59604 LUMO: 0.62858 factor:1 | 1 (-1.40095) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87308 HOMO: -6.45998 LUMO: -0.61770 factor:1 | 1 (-0.95523) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81719 HOMO: -6.75659 LUMO: -0.34014 factor:1 | 1 (-0.89934) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.95030 HOMO: -6.63958 LUMO: 0.36191 factor:1 | 1 (-1.03245) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61810 HOMO: -5.92936 LUMO: -0.67484 factor:1 | 1 (-1.70025) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.74714 HOMO: -5.67630 LUMO: 1.80956 factor:1 | 1 (-0.82929) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.44647 HOMO: -6.50352 LUMO: -0.78369 factor:1 | 1 (-2.52862) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.30192 HOMO: -6.35930 LUMO: -0.75648 factor:1 | 1 (-2.38407) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.81203 HOMO: -6.74298 LUMO: 0.48980 factor:1 | 1 (-1.89418) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96301 HOMO: -6.85183 LUMO: 0.15510 factor:1 | 1 (-1.04516) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.86390 HOMO: -6.90897 LUMO: 0.26123 factor:1 | 1 (-1.94605) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.20078 HOMO: -6.85999 LUMO: 0.47892 factor:1 | 1 (-2.28293) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.52580 HOMO: -6.69944 LUMO: 0.57416 factor:1 | 1 (-1.60795) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.54095 HOMO: -6.74026 LUMO: 0.69933 factor:1 | 1 (-1.62310) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.91030 HOMO: -6.52801 LUMO: 0.75376 factor:1 | 1 (-1.99244) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.91674 HOMO: -7.05863 LUMO: 0.44627 factor:1 | 1 (-1.99889) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.98486 HOMO: -6.96339 LUMO: 0.48164 factor:1 | 1 (-1.06701) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.29735 HOMO: -6.95795 LUMO: 0.44355 factor:1 | 1 (-2.37950) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.57720 HOMO: -6.36746 LUMO: 0.58777 factor:1 | 1 (-1.65935) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.52457 HOMO: -6.69400 LUMO: 0.40545 factor:1 | 1 (-1.60672) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.86817 HOMO: -6.30760 LUMO: -0.66668 factor:1 | 1 (-1.95032) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.42028 HOMO: -6.53617 LUMO: -0.64491 factor:1 | 1 (-0.50243) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.51561 HOMO: -6.80829 LUMO: 0.17415 factor:1 | -1 (0.40224) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.07045 HOMO: -6.80285 LUMO: 0.73471 factor:1 | 1 (-0.15260) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.13884 HOMO: -6.43821 LUMO: 0.21769 factor:1 | 1 (-2.22099) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.15300 HOMO: -6.98788 LUMO: 0.10885 factor:1 | 1 (-1.23515) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.02703 HOMO: -7.15115 LUMO: 0.40817 factor:1 | 1 (-2.10918) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.13491 HOMO: -6.00011 LUMO: -0.98505 factor:1 | 1 (-1.21706) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.48446 HOMO: -6.16882 LUMO: -0.77825 factor:1 | 1 (-1.56661) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.61857 HOMO: -6.30760 LUMO: 0.34831 factor:1 | 1 (-0.70072) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.75225 HOMO: -6.64502 LUMO: 0.63403 factor:1 | 1 (-1.83440) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.53881 HOMO: -6.93618 LUMO: 0.96600 factor:1 | 1 (-1.62096) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.66946 HOMO: -6.45182 LUMO: 0.16327 factor:1 | 1 (-0.75161) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.39054 HOMO: -6.99605 LUMO: 0.20953 factor:1 | 1 (-0.47269) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.98159 HOMO: -6.72665 LUMO: 0.32654 factor:1 | 1 (-2.06374) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87452 HOMO: -6.38379 LUMO: 0.45443 factor:1 | 1 (-0.95667) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36873 HOMO: -6.65318 LUMO: 0.04354 factor:1 | 1 (-1.45088) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80481 HOMO: -6.94707 LUMO: -1.68438 factor:1 | 1 (-0.88696) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60643 HOMO: -6.71849 LUMO: 0.15783 factor:1 | 1 (-0.68858) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.65695 HOMO: -6.97156 LUMO: 0.43266 factor:1 | -1 (0.26090) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79799 HOMO: -6.91441 LUMO: -0.54695 factor:1 | 1 (-1.88014) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.08130 HOMO: -6.74842 LUMO: -0.76192 factor:1 | 1 (-1.16345) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.63021 HOMO: -6.70489 LUMO: 0.19048 factor:1 | 1 (-1.71236) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.38437 HOMO: -7.25728 LUMO: 0.33470 factor:1 | -1 (0.53348) | 1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.10922 HOMO: -6.96339 LUMO: 0.55511 factor:1 | 1 (-1.19137) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14674 HOMO: -6.77564 LUMO: 0.72382 factor:1 | 1 (-1.22889) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.17071 HOMO: -6.75387 LUMO: 0.39729 factor:1 | -1 (0.74714) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.93507 HOMO: -7.00149 LUMO: 0.06531 factor:1 | 1 (-1.01722) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23368 HOMO: -7.09945 LUMO: 0.33470 factor:1 | 1 (-1.31583) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17439 HOMO: -7.20830 LUMO: 0.59593 factor:1 | 1 (-1.25654) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.16519 HOMO: -6.40556 LUMO: 0.56600 factor:1 | 1 (-1.24734) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.67919 HOMO: -6.77291 LUMO: 0.73471 factor:1 | -1 (1.23866) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57460 HOMO: -6.65046 LUMO: 0.09796 factor:1 | 1 (-0.65675) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.61140 HOMO: -6.95795 LUMO: 0.22313 factor:1 | -1 (0.30645) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.90023 HOMO: -6.85727 LUMO: 0.04626 factor:1 | -1 (1.01762) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88843 HOMO: -7.27360 LUMO: 0.42178 factor:1 | 1 (-0.97058) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.19913 HOMO: -6.78924 LUMO: -0.13334 factor:1 | 1 (-1.28128) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.75618 HOMO: -6.63141 LUMO: 0.38368 factor:1 | 1 (-0.83833) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.92394 HOMO: -6.92258 LUMO: 0.39184 factor:1 | 1 (-1.00609) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.42717 HOMO: -6.19331 LUMO: -0.46804 factor:1 | 1 (-0.50932) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.50350 HOMO: -7.26544 LUMO: -0.05442 factor:1 | -1 (0.41435) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.55722 HOMO: -7.09401 LUMO: 0.30749 factor:1 | -1 (0.36063) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.22442 HOMO: -6.14705 LUMO: -0.88709 factor:1 | -1 (0.69343) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.31417 HOMO: -6.53617 LUMO: -0.28572 factor:1 | -1 (0.60368) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52616 HOMO: -6.37291 LUMO: -0.67212 factor:1 | 1 (-0.60831) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.67061 HOMO: -6.65591 LUMO: 0.03810 factor:1 | -1 (0.24724) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.37283 HOMO: -7.11034 LUMO: 0.75103 factor:1 | -1 (0.54502) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.92392 HOMO: -6.85183 LUMO: -0.05987 factor:1 | 1 (-0.00607) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.71513 HOMO: -6.70761 LUMO: -0.05442 factor:1 | 1 (-1.79728) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05575 HOMO: -6.23413 LUMO: 0.06259 factor:1 | 1 (-1.13790) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.81818 HOMO: -6.55794 LUMO: 0.74015 factor:1 | 1 (-1.90033) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.29227 HOMO: -7.27905 LUMO: 0.26939 factor:1 | 1 (-1.37442) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.08797 HOMO: -6.34842 LUMO: -0.86804 factor:1 | 1 (-1.17012) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.19039 HOMO: -6.27222 LUMO: 1.46125 factor:1 | 1 (-1.27254) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.74292 HOMO: -6.65046 LUMO: 2.04902 factor:1 | 1 (-1.82507) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14408 HOMO: -7.11850 LUMO: -1.14016 factor:1 | 1 (-1.22623) | 1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14500 HOMO: -6.88720 LUMO: -1.20274 factor:1 | 1 (-1.22715) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80105 HOMO: -6.69400 LUMO: -0.31565 factor:1 | 1 (-0.88320) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.92046 HOMO: -6.95523 LUMO: -1.55377 factor:1 | 1 (-0.00261) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.03678 HOMO: -6.41372 LUMO: -0.83539 factor:1 | 1 (-1.11893) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81645 HOMO: -6.13889 LUMO: -0.90070 factor:1 | 1 (-0.89860) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11678 HOMO: -6.44366 LUMO: -0.55511 factor:1 | 1 (-1.19893) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.27583 HOMO: -6.10079 LUMO: -0.71022 factor:1 | 1 (-1.35798) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11510 HOMO: -6.90353 LUMO: -0.64763 factor:1 | 1 (-1.19725) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.07253 HOMO: -6.65046 LUMO: -0.82450 factor:1 | -1 (0.84532) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.47333 HOMO: -6.81645 LUMO: -0.85444 factor:1 | 1 (-1.55548) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.31834 HOMO: -6.20692 LUMO: 1.30887 factor:1 | 1 (-1.40049) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81762 HOMO: -5.96201 LUMO: 1.33880 factor:1 | 1 (-0.89977) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.04264 HOMO: -6.52529 LUMO: 1.58914 factor:1 | 1 (-0.12479) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.27992 HOMO: -6.58516 LUMO: 1.97555 factor:1 | 1 (-1.36207) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.02307 HOMO: -6.84366 LUMO: 0.15783 factor:1 | 1 (-1.10522) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01436 HOMO: -6.45726 LUMO: 0.42994 factor:1 | 1 (-1.09651) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.10908 HOMO: -6.75387 LUMO: 0.14422 factor:1 | 1 (-1.19123) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62080 HOMO: -6.69944 LUMO: 1.79051 factor:1 | 1 (-0.70295) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.99608 HOMO: -6.59876 LUMO: 1.90208 factor:1 | 1 (-0.07823) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.32343 HOMO: -7.05863 LUMO: 1.20819 factor:1 | 1 (-1.40558) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45862 HOMO: -6.54978 LUMO: 2.01636 factor:1 | 1 (-0.54077) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23709 HOMO: -5.52119 LUMO: 1.95106 factor:1 | 1 (-1.31924) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57179 HOMO: -6.53617 LUMO: 1.60275 factor:1 | 1 (-0.65394) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62692 HOMO: -6.11440 LUMO: 1.89119 factor:1 | 1 (-0.70907) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.66762 HOMO: -7.31986 LUMO: 0.48708 factor:1 | 1 (-1.74977) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.33769 HOMO: -6.76475 LUMO: -0.75648 factor:1 | 1 (-1.41984) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.65840 HOMO: -6.76747 LUMO: -1.06941 factor:1 | 1 (-1.74055) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.84625 HOMO: -6.87087 LUMO: 0.72927 factor:1 | 1 (-0.92840) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.51625 HOMO: -7.00965 LUMO: 0.02177 factor:1 | 1 (-1.59840) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79691 HOMO: -6.54706 LUMO: -0.03265 factor:1 | 1 (-1.87906) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05637 HOMO: -6.62325 LUMO: -0.63675 factor:1 | 1 (-1.13852) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.95108 HOMO: -7.03414 LUMO: -1.24084 factor:1 | 1 (-2.03323) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.98037 HOMO: -7.04503 LUMO: -0.10068 factor:1 | 1 (-1.06252) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.92230 HOMO: -6.67223 LUMO: 0.03537 factor:1 | 1 (-2.00445) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.69157 HOMO: -6.82734 LUMO: 0.58777 factor:1 | 1 (-1.77372) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87253 HOMO: -6.84366 LUMO: 0.46531 factor:1 | 1 (-0.95468) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.53285 HOMO: -7.03959 LUMO: -1.15104 factor:1 | 1 (-1.61500) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01246 HOMO: -6.91169 LUMO: -0.41361 factor:1 | 1 (-1.09461) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.58158 HOMO: -7.10217 LUMO: -0.44627 factor:1 | 1 (-1.66373) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.74490 HOMO: -6.88176 LUMO: -0.19592 factor:1 | 1 (-1.82705) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.63998 HOMO: -7.21374 LUMO: -0.46531 factor:1 | 1 (-1.72213) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.26777 HOMO: -6.54978 LUMO: 0.16871 factor:1 | -1 (0.65008) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.63481 HOMO: -6.71305 LUMO: -0.13061 factor:1 | 1 (-1.71696) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64986 HOMO: -6.74842 LUMO: -0.36191 factor:1 | 1 (-0.73201) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06514 HOMO: -6.74570 LUMO: -0.09796 factor:1 | 1 (-1.14729) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.72399 HOMO: -6.93890 LUMO: -0.27211 factor:1 | 1 (-0.80614) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11714 HOMO: -6.88720 LUMO: -0.18776 factor:1 | 1 (-1.19929) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.13058 HOMO: -6.74842 LUMO: 0.02993 factor:1 | 1 (-1.21273) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96761 HOMO: -6.70216 LUMO: 0.01361 factor:1 | 1 (-1.04976) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06587 HOMO: -6.90625 LUMO: 0.00544 factor:1 | 1 (-1.14802) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.28364 HOMO: -6.18243 LUMO: 0.25851 factor:1 | 1 (-1.36579) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.22283 HOMO: -6.32937 LUMO: -0.20953 factor:1 | 1 (-1.30498) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30511 HOMO: -6.78108 LUMO: 0.00544 factor:1 | 1 (-1.38726) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.37377 HOMO: -5.97562 LUMO: 0.28572 factor:1 | 1 (-1.45592) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89798 HOMO: -5.97290 LUMO: -0.18504 factor:1 | 1 (-0.98013) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.44737 HOMO: -6.12800 LUMO: 0.42178 factor:1 | 1 (-1.52952) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.29942 HOMO: -6.24229 LUMO: -0.00816 factor:1 | -1 (0.61843) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89858 HOMO: -6.61781 LUMO: 0.12789 factor:1 | 1 (-0.98073) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52850 HOMO: -6.70489 LUMO: 0.14694 factor:1 | 1 (-0.61065) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.60209 HOMO: -6.86543 LUMO: -0.21225 factor:1 | -1 (0.31576) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.37032 HOMO: -6.90081 LUMO: -0.20136 factor:1 | 1 (-0.45247) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88788 HOMO: -7.12938 LUMO: -0.25851 factor:1 | 1 (-0.97003) | 1 | 1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.38795 HOMO: -6.93074 LUMO: -0.26667 factor:1 | 1 (-1.47010) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.37668 HOMO: -7.00421 LUMO: -0.31021 factor:1 | 1 (-1.45883) | -1 | -1 |
| G: -6694.55216 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.67181 HOMO: -7.10761 LUMO: -0.17415 factor:1 | 1 (-1.75396) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85602 HOMO: -8.21240 LUMO: 0.05987 factor:1 | 1 (-0.93817) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.72486 HOMO: -7.14843 LUMO: -0.46531 factor:1 | 1 (-0.80701) | 1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.78096 HOMO: -6.80829 LUMO: -0.29933 factor:1 | 1 (-1.86311) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.86829 HOMO: -6.84094 LUMO: -0.53606 factor:1 | 1 (-0.95044) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.64338 HOMO: -6.81917 LUMO: -0.26667 factor:1 | 1 (-1.72553) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59332 HOMO: -6.85727 LUMO: -1.20002 factor:1 | 1 (-0.67547) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.65383 HOMO: -6.39468 LUMO: -1.06941 factor:1 | 1 (-1.73598) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.12617 HOMO: -6.00827 LUMO: -1.94017 factor:1 | 1 (-1.20832) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.99953 HOMO: -6.80829 LUMO: 0.18504 factor:1 | 1 (-1.08168) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.34129 HOMO: -6.54434 LUMO: -0.95784 factor:1 | 1 (-0.42344) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.00239 HOMO: -6.45454 LUMO: -0.07347 factor:1 | 1 (-1.08454) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.44245 HOMO: -5.33887 LUMO: 1.11839 factor:1 | 1 (-1.52460) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.46150 HOMO: -5.75249 LUMO: 0.70477 factor:1 | 1 (-1.54365) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.68420 HOMO: -5.64092 LUMO: 0.87076 factor:1 | 1 (-1.76635) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.42294 HOMO: -5.14295 LUMO: 1.06124 factor:1 | 1 (-1.50509) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.43369 HOMO: -5.05043 LUMO: 1.21091 factor:1 | 1 (-1.51584) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.70158 HOMO: -5.05588 LUMO: 1.02859 factor:1 | 1 (-1.78373) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.46052 HOMO: -5.76337 LUMO: 0.79457 factor:1 | 1 (-1.54267) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64154 HOMO: -5.01506 LUMO: 1.00138 factor:1 | 1 (-0.72369) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20498 HOMO: -4.84363 LUMO: 1.53744 factor:1 | 1 (-1.28713) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.31916 HOMO: -5.17833 LUMO: 1.45309 factor:1 | 1 (-0.40131) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.65620 HOMO: -5.13751 LUMO: 0.51157 factor:1 | 1 (-0.73835) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.68316 HOMO: -5.56473 LUMO: 0.32109 factor:1 | 1 (-1.76531) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.87035 HOMO: -4.69941 LUMO: 1.14016 factor:1 | 1 (-1.95250) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81776 HOMO: -4.49260 LUMO: 1.86398 factor:1 | 1 (-0.89991) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46567 HOMO: -4.32117 LUMO: 1.68438 factor:1 | 1 (-0.54782) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.11546 HOMO: -4.44906 LUMO: 1.37690 factor:1 | 1 (-0.19761) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.47336 HOMO: -4.62049 LUMO: 1.34968 factor:1 | 1 (-1.55551) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06737 HOMO: -4.59600 LUMO: 1.58370 factor:1 | 1 (-1.14952) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.73215 HOMO: -4.98785 LUMO: 1.46669 factor:1 | 1 (-0.81430) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58045 HOMO: -5.06676 LUMO: 1.27349 factor:1 | 1 (-0.66260) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.13409 HOMO: -5.09125 LUMO: 1.13471 factor:1 | 1 (-1.21624) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.21979 HOMO: -4.84635 LUMO: 1.33608 factor:1 | 1 (-0.30194) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23001 HOMO: -4.94431 LUMO: 1.18370 factor:1 | 1 (-1.31216) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91504 HOMO: -4.92526 LUMO: 1.39867 factor:1 | 1 (-0.99719) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60785 HOMO: -5.71983 LUMO: 0.60137 factor:1 | 1 (-0.69000) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50901 HOMO: -5.10486 LUMO: 1.05580 factor:1 | 1 (-1.59116) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.43694 HOMO: -5.20282 LUMO: 1.01226 factor:1 | -1 (0.48091) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64148 HOMO: -4.98513 LUMO: 1.53744 factor:1 | 1 (-0.72363) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06745 HOMO: -5.67085 LUMO: 0.17687 factor:1 | 1 (-1.14960) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.52240 HOMO: -5.87222 LUMO: 0.12517 factor:1 | 1 (-1.60455) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.99615 HOMO: -5.20826 LUMO: 0.91702 factor:1 | 1 (-2.07830) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.96638 HOMO: -5.94569 LUMO: 0.63130 factor:1 | 1 (-2.04853) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.67364 HOMO: -5.35792 LUMO: 0.91430 factor:1 | 1 (-1.75579) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.03794 HOMO: -5.36336 LUMO: 1.44220 factor:1 | 1 (-2.12009) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.34053 HOMO: -5.83412 LUMO: 0.71294 factor:1 | 1 (-2.42268) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.76482 HOMO: -4.97696 LUMO: 1.72792 factor:1 | 1 (-1.84697) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.23849 HOMO: -5.55929 LUMO: 0.23130 factor:1 | 1 (-2.32064) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.63066 HOMO: -5.71167 LUMO: 0.47348 factor:1 | 1 (-2.71281) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.26897 HOMO: -7.31986 LUMO: -2.54699 factor:1 | 1 (-2.35112) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76568 HOMO: -5.34704 LUMO: 1.19730 factor:1 | 1 (-0.84783) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.55027 HOMO: -5.45860 LUMO: 0.80818 factor:1 | 1 (-0.63242) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58080 HOMO: -5.12663 LUMO: 1.20274 factor:1 | 1 (-0.66295) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.98884 HOMO: -5.37153 LUMO: 1.05580 factor:1 | 1 (-0.07099) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79388 HOMO: -5.47221 LUMO: 0.97961 factor:1 | 1 (-1.87603) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89009 HOMO: -5.06948 LUMO: 1.12111 factor:1 | 1 (-0.97224) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.38101 HOMO: -5.19737 LUMO: 1.25444 factor:1 | 1 (-1.46316) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.28739 HOMO: -5.27901 LUMO: 1.00682 factor:1 | 1 (-2.36954) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.73369 HOMO: -5.38513 LUMO: 0.49253 factor:1 | 1 (-1.81584) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.37131 HOMO: -5.12390 LUMO: 1.22995 factor:1 | 1 (-2.45346) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.40278 HOMO: -5.31438 LUMO: 0.70205 factor:1 | 1 (-1.48493) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.78635 HOMO: -5.17561 LUMO: 1.04492 factor:1 | 1 (-1.86850) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.00843 HOMO: -4.94431 LUMO: 1.52656 factor:1 | 1 (-1.09058) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85730 HOMO: -5.13751 LUMO: 0.93879 factor:1 | 1 (-0.93945) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.74374 HOMO: -5.49942 LUMO: 0.97689 factor:1 | 1 (-0.82589) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.49966 HOMO: -5.79058 LUMO: 0.53879 factor:1 | 1 (-0.58181) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52156 HOMO: -5.36881 LUMO: 1.56465 factor:1 | 1 (-0.60371) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69710 HOMO: -4.67492 LUMO: 1.32792 factor:1 | 1 (-0.77925) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.56265 HOMO: -4.60145 LUMO: 1.19458 factor:1 | 1 (-0.64480) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.08860 HOMO: -4.49260 LUMO: 1.60547 factor:1 | 1 (-0.17075) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91175 HOMO: -4.65043 LUMO: 1.34696 factor:1 | 1 (-0.99390) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.04214 HOMO: -4.77560 LUMO: 1.35241 factor:1 | 1 (-1.12429) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70782 HOMO: -4.94431 LUMO: 1.17825 factor:1 | 1 (-0.78997) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52477 HOMO: -4.87084 LUMO: 1.41771 factor:1 | 1 (-0.60692) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.56113 HOMO: -5.34432 LUMO: 1.16737 factor:1 | 1 (-0.64328) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.96860 HOMO: -4.94975 LUMO: 1.67622 factor:1 | 1 (-0.05075) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.39513 HOMO: -4.81369 LUMO: 1.14288 factor:1 | 1 (-1.47728) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30302 HOMO: -5.22459 LUMO: 0.29660 factor:1 | 1 (-1.38517) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.71576 HOMO: -5.21642 LUMO: 0.37824 factor:1 | 1 (-1.79791) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.99762 HOMO: -5.00417 LUMO: 1.01226 factor:1 | 1 (-2.07977) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.71475 HOMO: -5.46677 LUMO: 0.10612 factor:1 | 1 (-2.79690) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.00222 HOMO: -5.51303 LUMO: 0.54151 factor:1 | 1 (-2.08436) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.56903 HOMO: -5.63004 LUMO: 0.17960 factor:1 | 1 (-2.65118) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14680 HOMO: -4.79193 LUMO: 1.12111 factor:1 | 1 (-1.22895) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.72518 HOMO: -5.43411 LUMO: 0.45987 factor:1 | 1 (-1.80733) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.71633 HOMO: -7.06135 LUMO: -2.13881 factor:1 | 1 (-1.79848) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50887 HOMO: -5.33071 LUMO: 1.14016 factor:1 | 1 (-1.59102) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79271 HOMO: -7.12394 LUMO: -0.03810 factor:1 | 1 (-1.87486) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.18244 HOMO: -7.20558 LUMO: -2.50889 factor:1 | 1 (-2.26459) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.10341 HOMO: -7.26816 LUMO: -2.11432 factor:1 | 1 (-2.18556) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.09871 HOMO: -7.89674 LUMO: 0.31021 factor:1 | 1 (-2.18086) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.03749 HOMO: -7.26544 LUMO: 0.22858 factor:1 | 1 (-1.11964) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06182 HOMO: -7.12666 LUMO: -0.02449 factor:1 | 1 (-1.14397) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.56015 HOMO: -7.68722 LUMO: 0.71838 factor:1 | 1 (-0.64230) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.71044 HOMO: -6.86271 LUMO: -0.96056 factor:1 | 1 (-0.79259) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06837 HOMO: -7.07496 LUMO: -1.11839 factor:1 | 1 (-1.15052) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.00930 HOMO: -7.06952 LUMO: -2.08439 factor:1 | 1 (-1.09145) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58905 HOMO: -6.60965 LUMO: -2.11977 factor:1 | 1 (-0.67120) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62431 HOMO: -6.87360 LUMO: -1.85854 factor:1 | 1 (-0.70646) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77846 HOMO: -7.67089 LUMO: -0.24762 factor:1 | 1 (-0.86061) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.12867 HOMO: -6.45726 LUMO: -1.86398 factor:1 | 1 (-2.21082) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.09098 HOMO: -6.91713 LUMO: 0.33198 factor:1 | 1 (-2.17313) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.49044 HOMO: -6.83278 LUMO: 0.26667 factor:1 | 1 (-2.57259) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.65080 HOMO: -6.89264 LUMO: -1.00682 factor:1 | 1 (-2.73295) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.52835 HOMO: -6.57427 LUMO: 0.22041 factor:1 | 1 (-2.61050) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.36824 HOMO: -7.52123 LUMO: -0.01905 factor:1 | 1 (-2.45039) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.68802 HOMO: -7.37429 LUMO: -0.08980 factor:1 | 1 (-2.77017) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.67687 HOMO: -7.28449 LUMO: -0.26395 factor:1 | 1 (-2.75902) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.73821 HOMO: -6.79740 LUMO: -0.60954 factor:1 | 1 (-1.82036) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.48190 HOMO: -7.12666 LUMO: -0.60681 factor:1 | 1 (-2.56405) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.88447 HOMO: -6.96611 LUMO: -0.30477 factor:1 | 1 (-1.96662) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.04639 HOMO: -7.08040 LUMO: -0.31293 factor:1 | 1 (-1.12854) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05444 HOMO: -6.78924 LUMO: -0.73743 factor:1 | 1 (-1.13659) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58086 HOMO: -7.57293 LUMO: -1.11295 factor:1 | 1 (-0.66301) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68521 HOMO: -7.15932 LUMO: -0.23130 factor:1 | 1 (-0.76736) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.53095 HOMO: -7.48585 LUMO: -0.10068 factor:1 | 1 (-0.61310) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.34662 HOMO: -7.17020 LUMO: -0.26123 factor:1 | 1 (-0.42877) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17540 HOMO: -7.43143 LUMO: -0.16055 factor:1 | 1 (-1.25755) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.17830 HOMO: -7.14843 LUMO: -0.10612 factor:1 | 1 (-2.26045) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.32792 HOMO: -6.95523 LUMO: -0.22585 factor:1 | 1 (-1.41007) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.05574 HOMO: -7.06680 LUMO: -0.51974 factor:1 | 1 (-2.13789) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.31724 HOMO: -6.80829 LUMO: -0.64763 factor:1 | 1 (-2.39939) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.46084 HOMO: -7.13210 LUMO: -0.48164 factor:1 | 1 (-1.54299) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.31924 HOMO: -7.16204 LUMO: -0.45715 factor:1 | 1 (-1.40139) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.01220 HOMO: -7.15115 LUMO: -0.43266 factor:1 | 1 (-2.09435) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50452 HOMO: -7.15932 LUMO: -2.52794 factor:1 | 1 (-1.58667) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.66818 HOMO: -7.21102 LUMO: -2.65311 factor:1 | 1 (-0.75033) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.72578 HOMO: -6.57427 LUMO: -2.78645 factor:1 | 1 (-0.80793) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.63538 HOMO: -6.40828 LUMO: -3.23815 factor:1 | 1 (-1.71753) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.04173 HOMO: -7.71987 LUMO: -0.20953 factor:1 | 1 (-2.12388) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79759 HOMO: -7.47769 LUMO: -0.43810 factor:1 | 1 (-1.87974) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76706 HOMO: -6.68040 LUMO: -2.22589 factor:1 | 1 (-0.84921) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59792 HOMO: -6.92802 LUMO: -1.99187 factor:1 | 1 (-0.68007) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.70390 HOMO: -7.73620 LUMO: 0.01633 factor:1 | 1 (-1.78605) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.78368 HOMO: -7.28721 LUMO: -0.18504 factor:1 | 1 (-1.86583) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.42952 HOMO: -7.49674 LUMO: -0.19864 factor:1 | 1 (-1.51167) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.76266 HOMO: -7.10489 LUMO: -2.56331 factor:1 | -1 (0.15519) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.66984 HOMO: -7.36612 LUMO: 0.16055 factor:1 | 1 (-0.75199) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.37815 HOMO: -7.67633 LUMO: 0.33198 factor:1 | 1 (-1.46030) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.51881 HOMO: -7.07768 LUMO: -0.27483 factor:1 | 1 (-0.60096) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.91049 HOMO: -7.32531 LUMO: 0.05442 factor:1 | 1 (-1.99264) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.07384 HOMO: -6.79740 LUMO: -1.21635 factor:1 | 1 (-2.15599) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45810 HOMO: -7.14027 LUMO: 0.12517 factor:1 | 1 (-0.54025) | 1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61617 HOMO: -7.17292 LUMO: 0.16871 factor:1 | 1 (-1.69832) | 1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.04017 HOMO: -7.08312 LUMO: -1.38778 factor:1 | 1 (-0.12232) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.30123 HOMO: -6.75387 LUMO: -1.88031 factor:1 | 1 (-0.38338) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.87318 HOMO: -7.07768 LUMO: -1.25717 factor:1 | 1 (-1.95533) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.45252 HOMO: -6.46543 LUMO: -1.14016 factor:1 | 1 (-1.53467) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.04880 HOMO: -7.37973 LUMO: -0.45987 factor:1 | 1 (-2.13095) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.59189 HOMO: -7.46408 LUMO: 0.03265 factor:1 | 1 (-1.67404) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.77973 HOMO: -7.96477 LUMO: -0.19864 factor:1 | 1 (-1.86188) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17442 HOMO: -6.93890 LUMO: -1.11839 factor:1 | 1 (-1.25657) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57982 HOMO: -7.06408 LUMO: -1.08846 factor:1 | 1 (-0.66197) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68630 HOMO: -7.14027 LUMO: -0.33470 factor:1 | 1 (-0.76845) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.45831 HOMO: -7.38245 LUMO: 0.10885 factor:1 | 1 (-1.54046) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.28711 HOMO: -7.59470 LUMO: -1.21363 factor:1 | 1 (-0.36926) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58747 HOMO: -7.23279 LUMO: -1.23812 factor:1 | 1 (-0.66962) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.86653 HOMO: -6.90897 LUMO: 0.23402 factor:1 | -1 (0.05132) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88976 HOMO: -7.36340 LUMO: -0.17143 factor:1 | 1 (-0.97191) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.37310 HOMO: -6.61781 LUMO: -0.01361 factor:1 | 1 (-0.45525) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96312 HOMO: -6.80013 LUMO: 0.38368 factor:1 | 1 (-1.04527) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.02123 HOMO: -6.72121 LUMO: -0.95512 factor:1 | 1 (-0.10338) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.71464 HOMO: -6.24773 LUMO: -0.69933 factor:1 | -1 (0.20321) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69629 HOMO: -6.56883 LUMO: 0.14694 factor:1 | 1 (-0.77844) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.92206 HOMO: -6.51441 LUMO: -1.27621 factor:1 | 1 (-1.00421) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27024 HOMO: -6.91986 LUMO: -1.16737 factor:1 | 1 (-0.35239) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.98675 HOMO: -6.17971 LUMO: -0.65307 factor:1 | 1 (-0.06890) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69751 HOMO: -7.22462 LUMO: 0.04354 factor:1 | 1 (-0.77966) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05039 HOMO: -7.16204 LUMO: -0.23674 factor:1 | 1 (-1.13254) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.62327 HOMO: -6.81645 LUMO: -0.19320 factor:1 | 1 (-1.70542) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88383 HOMO: -6.69400 LUMO: 0.04082 factor:1 | 1 (-0.96598) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.55737 HOMO: -6.63141 LUMO: -0.22858 factor:1 | 1 (-0.63952) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.26983 HOMO: -6.92258 LUMO: -1.11295 factor:1 | 1 (-0.35198) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59345 HOMO: -6.60148 LUMO: -1.13744 factor:1 | 1 (-0.67560) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46572 HOMO: -6.78108 LUMO: -0.82450 factor:1 | 1 (-0.54787) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70061 HOMO: -7.05591 LUMO: -0.97145 factor:1 | 1 (-0.78276) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81909 HOMO: -6.65318 LUMO: -1.26261 factor:1 | 1 (-0.90124) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.02703 HOMO: -6.98244 LUMO: -0.98233 factor:1 | 1 (-2.10918) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.29177 HOMO: -7.11850 LUMO: -0.99594 factor:1 | 1 (-2.37392) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61236 HOMO: -6.64230 LUMO: -0.93879 factor:1 | 1 (-1.69451) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36473 HOMO: -6.62053 LUMO: -1.22451 factor:1 | 1 (-1.44688) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77212 HOMO: -7.02598 LUMO: -0.85172 factor:1 | 1 (-0.85427) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.24160 HOMO: -7.06680 LUMO: -0.89253 factor:1 | 1 (-1.32375) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.66635 HOMO: -7.17292 LUMO: 0.00272 factor:1 | 1 (-0.74850) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27451 HOMO: -7.03142 LUMO: -0.35103 factor:1 | 1 (-0.35666) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05463 HOMO: -6.96884 LUMO: -0.09796 factor:1 | 1 (-1.13678) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58706 HOMO: -6.56339 LUMO: -0.99322 factor:1 | 1 (-0.66921) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81041 HOMO: -7.08857 LUMO: -0.17687 factor:1 | 1 (-0.89256) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.75579 HOMO: -7.05863 LUMO: -0.22041 factor:1 | 1 (-1.83794) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.23822 HOMO: -7.15115 LUMO: -0.17960 factor:1 | 1 (-2.32037) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.67630 HOMO: -6.67495 LUMO: -0.96600 factor:1 | 1 (-1.75845) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.47872 HOMO: -6.74026 LUMO: -1.79867 factor:1 | 1 (-1.56087) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.69481 HOMO: -6.73482 LUMO: -1.78235 factor:1 | 1 (-1.77696) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27119 HOMO: -6.09807 LUMO: 0.16871 factor:1 | 1 (-0.35334) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.04114 HOMO: -6.72393 LUMO: 0.27211 factor:1 | 1 (-0.12329) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.31160 HOMO: -6.40556 LUMO: -0.04354 factor:1 | 1 (-0.39375) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.42537 HOMO: -6.56883 LUMO: 0.22041 factor:1 | 1 (-0.50752) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.24509 HOMO: -7.22462 LUMO: 0.15783 factor:1 | 1 (-0.32724) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.26678 HOMO: -6.83550 LUMO: 0.19320 factor:1 | 1 (-0.34893) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.22085 HOMO: -7.26816 LUMO: -0.07619 factor:1 | 1 (-0.30300) | 1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79440 HOMO: -7.13483 LUMO: 0.33198 factor:1 | 1 (-1.87655) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80168 HOMO: -6.58243 LUMO: -0.26395 factor:1 | 1 (-0.88383) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.37692 HOMO: -7.38517 LUMO: 0.17143 factor:1 | 1 (-2.45907) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.64773 HOMO: -6.80013 LUMO: 0.25851 factor:1 | 1 (-1.72988) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.39358 HOMO: -6.96611 LUMO: 0.11429 factor:1 | 1 (-1.47573) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.70537 HOMO: -6.51713 LUMO: -1.14560 factor:1 | 1 (-1.78752) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.38289 HOMO: -7.15387 LUMO: -0.35647 factor:1 | 1 (-0.46504) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.43651 HOMO: -5.26540 LUMO: 1.26805 factor:1 | -1 (0.48134) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.10047 HOMO: -6.76475 LUMO: -0.16327 factor:1 | 1 (-0.18262) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.40044 HOMO: -6.55250 LUMO: -0.71838 factor:1 | 1 (-1.48259) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.56842 HOMO: -6.76203 LUMO: -1.08301 factor:1 | 1 (-0.65057) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.37214 HOMO: -7.14027 LUMO: -0.01633 factor:1 | 1 (-0.45429) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.12261 HOMO: -6.94979 LUMO: -0.93879 factor:1 | 1 (-1.20476) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.18441 HOMO: -6.74842 LUMO: 0.31293 factor:1 | 1 (-0.26656) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.38574 HOMO: -6.43821 LUMO: 0.05987 factor:1 | 1 (-1.46789) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.49870 HOMO: -6.60420 LUMO: 0.22585 factor:1 | 1 (-0.58085) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.32858 HOMO: -6.43821 LUMO: 0.05987 factor:1 | 1 (-0.41073) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11670 HOMO: -6.34570 LUMO: 1.43948 factor:1 | 1 (-1.19885) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.55808 HOMO: -6.03004 LUMO: 1.21363 factor:1 | 1 (-0.64023) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.15156 HOMO: -6.68040 LUMO: -0.92247 factor:1 | 1 (-1.23371) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.25738 HOMO: -6.92530 LUMO: -0.31293 factor:1 | -1 (1.66047) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.97332 HOMO: -6.94979 LUMO: -0.19864 factor:1 | -1 (0.94453) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.61589 HOMO: -6.80829 LUMO: -0.30477 factor:1 | -1 (1.30196) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.92113 HOMO: -7.22734 LUMO: -1.02859 factor:1 | 1 (-1.00328) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45740 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-0.53955) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.13640 HOMO: -7.27088 LUMO: -0.78097 factor:1 | 1 (-1.21855) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.99145 HOMO: -7.29809 LUMO: -0.97145 factor:1 | 1 (-1.07360) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.61928 HOMO: -7.18925 LUMO: -0.94696 factor:1 | 1 (-0.70143) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.36964 HOMO: -7.33891 LUMO: -0.96873 factor:1 | 1 (-0.45179) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.02307 HOMO: -7.36068 LUMO: -0.28028 factor:1 | 1 (-1.10522) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.13224 HOMO: -7.10761 LUMO: -1.14832 factor:1 | 1 (-1.21439) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.04271 HOMO: -6.94707 LUMO: -0.65307 factor:1 | 1 (-1.12486) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.10205 HOMO: -6.91713 LUMO: -1.81228 factor:1 | -1 (0.81580) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76168 HOMO: -6.78652 LUMO: -2.01636 factor:1 | 1 (-0.84383) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.64851 HOMO: -6.52801 LUMO: -1.17553 factor:1 | -1 (0.26934) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.11824 HOMO: -7.54844 LUMO: -1.18642 factor:1 | 1 (-2.20039) | 1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23907 HOMO: -7.52939 LUMO: -1.23812 factor:1 | 1 (-1.32122) | 1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.98208 HOMO: -7.94572 LUMO: -0.81634 factor:1 | 1 (-2.06423) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.07852 HOMO: -7.55932 LUMO: -0.86260 factor:1 | 1 (-1.16067) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.09800 HOMO: -7.72259 LUMO: -1.39050 factor:1 | 1 (-2.18015) | 1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.22089 HOMO: -7.11850 LUMO: -1.01498 factor:1 | 1 (-1.30304) | 1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.69873 HOMO: -7.09673 LUMO: -1.00954 factor:1 | 1 (-1.78088) | 1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96549 HOMO: -6.06270 LUMO: 0.16327 factor:1 | 1 (-1.04764) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.20243 HOMO: -5.71167 LUMO: 0.70477 factor:1 | 1 (-0.28458) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.80620 HOMO: -5.38241 LUMO: 0.86260 factor:1 | -1 (0.11165) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58086 HOMO: -5.67357 LUMO: 1.27621 factor:1 | 1 (-0.66301) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.93403 HOMO: -7.56204 LUMO: -0.68573 factor:1 | 1 (-1.01618) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.57238 HOMO: -5.57833 LUMO: 1.13199 factor:1 | 1 (-1.65453) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.82689 HOMO: -7.58653 LUMO: -0.66124 factor:1 | 1 (-1.90904) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14043 HOMO: -7.91851 LUMO: -1.10206 factor:1 | 1 (-1.22258) | 1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80535 HOMO: -6.48992 LUMO: -1.00138 factor:1 | 1 (-0.88750) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.70413 HOMO: -7.09673 LUMO: -0.45171 factor:1 | -1 (0.21372) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.90834 HOMO: -6.63686 LUMO: 0.09252 factor:1 | 1 (-0.99049) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.22364 HOMO: -6.84366 LUMO: -0.14422 factor:1 | 1 (-1.30579) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.76828 HOMO: -6.93074 LUMO: 0.04354 factor:1 | -1 (1.14957) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.34349 HOMO: -6.90353 LUMO: -0.19864 factor:1 | 1 (-0.42564) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.94209 HOMO: -6.59876 LUMO: -0.10068 factor:1 | 1 (-1.02424) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.09998 HOMO: -6.74570 LUMO: -0.44627 factor:1 | 1 (-0.18213) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.76236 HOMO: -6.60148 LUMO: -0.61770 factor:1 | -1 (0.15549) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.63512 HOMO: -6.55794 LUMO: -1.06941 factor:1 | 1 (-0.71726) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69259 HOMO: -7.12666 LUMO: -0.11973 factor:1 | 1 (-0.77474) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58951 HOMO: -7.21646 LUMO: -0.50069 factor:1 | 1 (-0.67166) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.49040 HOMO: -7.27632 LUMO: -1.00682 factor:1 | 1 (-0.57255) | 1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.90218 HOMO: -6.74298 LUMO: 0.04354 factor:1 | -1 (0.01567) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85215 HOMO: -6.37291 LUMO: 0.14150 factor:1 | 1 (-0.93430) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.20697 HOMO: -5.61371 LUMO: 1.28438 factor:1 | 1 (-0.28912) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.07647 HOMO: -5.52119 LUMO: 0.99866 factor:1 | 1 (-0.15862) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62143 HOMO: -6.51985 LUMO: -0.10885 factor:1 | 1 (-0.70358) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.74631 HOMO: -5.61371 LUMO: 0.77280 factor:1 | -1 (0.17154) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01597 HOMO: -5.58922 LUMO: 0.24490 factor:1 | 1 (-1.09812) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.95011 HOMO: -6.32665 LUMO: -0.57144 factor:1 | 1 (-1.03226) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76018 HOMO: -6.29127 LUMO: -0.93607 factor:1 | 1 (-0.84233) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.89576 HOMO: -5.49670 LUMO: 0.27211 factor:1 | -1 (1.02209) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60935 HOMO: -5.68990 LUMO: 0.24218 factor:1 | 1 (-0.69150) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96617 HOMO: -5.68174 LUMO: 0.69933 factor:1 | 1 (-1.04832) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.09541 HOMO: -5.28173 LUMO: 1.00954 factor:1 | -1 (0.82244) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.08568 HOMO: -5.94025 LUMO: 0.73471 factor:1 | 1 (-1.16783) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.67724 HOMO: -5.65725 LUMO: 1.28710 factor:1 | 1 (-0.75939) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.58516 HOMO: -5.41507 LUMO: 0.87076 factor:1 | -1 (0.33269) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.33628 HOMO: -5.96474 LUMO: 0.29660 factor:1 | 1 (-0.41843) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.51972 HOMO: -7.00421 LUMO: 0.08708 factor:1 | -1 (0.39813) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.53351 HOMO: -5.40418 LUMO: 0.90070 factor:1 | 1 (-0.61566) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45198 HOMO: -7.00421 LUMO: -0.30477 factor:1 | 1 (-0.53413) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.37565 HOMO: -5.85861 LUMO: 0.74015 factor:1 | 1 (-0.45780) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.90829 HOMO: -5.71439 LUMO: 0.26395 factor:1 | 1 (-0.99044) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.67283 HOMO: -7.13755 LUMO: -0.78369 factor:1 | 1 (-0.75498) | 1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96062 HOMO: -7.31442 LUMO: -0.98233 factor:1 | 1 (-1.04277) | 1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.75634 HOMO: -7.25728 LUMO: -1.00410 factor:1 | 1 (-0.83849) | 1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.98609 HOMO: -7.48585 LUMO: -0.83811 factor:1 | 1 (-1.06824) | 1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.78306 HOMO: -7.24911 LUMO: -0.77280 factor:1 | 1 (-0.86521) | 1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.74805 HOMO: -7.55116 LUMO: -1.19730 factor:1 | -1 (0.16980) | 1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.53781 HOMO: -5.76881 LUMO: 0.28028 factor:1 | 1 (-0.61996) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.55896 HOMO: -5.77153 LUMO: -0.26939 factor:1 | -1 (0.35889) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.21162 HOMO: -5.82868 LUMO: 0.36735 factor:1 | 1 (-0.29377) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.28574 HOMO: -5.83140 LUMO: -0.17960 factor:1 | -1 (1.63211) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.93187 HOMO: -6.28855 LUMO: 0.01088 factor:1 | -1 (0.98598) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.64926 HOMO: -6.31576 LUMO: 0.25307 factor:1 | -1 (1.26859) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77901 HOMO: -7.06408 LUMO: -2.76196 factor:1 | 1 (-0.86116) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57408 HOMO: -5.95657 LUMO: 0.37552 factor:1 | 1 (-0.65623) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.82932 HOMO: -6.61781 LUMO: 0.02721 factor:1 | 1 (-0.91147) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.92955 HOMO: -6.26678 LUMO: -0.66668 factor:1 | 1 (-0.01170) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.78731 HOMO: -6.00011 LUMO: -0.13334 factor:1 | 1 (-0.86946) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69109 HOMO: -5.60555 LUMO: 0.67484 factor:1 | 1 (-0.77324) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.56336 HOMO: -5.79875 LUMO: 0.99049 factor:1 | 1 (-0.64551) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.97395 HOMO: -5.97834 LUMO: 0.48436 factor:1 | 1 (-1.05610) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89267 HOMO: -5.82868 LUMO: 0.91974 factor:1 | 1 (-0.97482) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.95294 HOMO: -5.86677 LUMO: 0.99594 factor:1 | 1 (-1.03509) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.19138 HOMO: -5.70079 LUMO: 0.48980 factor:1 | 1 (-0.27353) | -1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.25718 HOMO: -7.39605 LUMO: -1.02315 factor:1 | -1 (0.66067) | 1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.36872 HOMO: -7.22734 LUMO: -1.12927 factor:1 | 1 (-0.45087) | 1 | -1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.50075 HOMO: -7.58926 LUMO: -0.65035 factor:1 | -1 (0.41710) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46605 HOMO: -7.43959 LUMO: -0.75648 factor:1 | 1 (-0.54820) | 1 | 1 |
| G: -6694.55216 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.27861 HOMO: -7.55388 LUMO: -1.15104 factor:1 | 1 (-1.36076) | 1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.33692 HOMO: -6.74570 LUMO: -2.85447 factor:1 | 1 (-1.41907) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62004 HOMO: -7.35524 LUMO: -1.25444 factor:1 | 1 (-0.70219) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61992 HOMO: -6.81645 LUMO: -1.20819 factor:1 | 1 (-1.70207) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.92252 HOMO: -6.99605 LUMO: -1.62996 factor:1 | 1 (-1.00467) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.02664 HOMO: -6.88992 LUMO: -0.47620 factor:1 | 1 (-0.10879) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.61884 HOMO: -7.22190 LUMO: -0.01905 factor:1 | 1 (-0.70099) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.97738 HOMO: -6.77836 LUMO: -0.82995 factor:1 | 1 (-1.05953) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.94568 HOMO: -6.48447 LUMO: -0.95512 factor:1 | 1 (-1.02783) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.38009 HOMO: -7.81239 LUMO: 1.22179 factor:1 | 1 (-0.46224) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.65612 HOMO: -7.36612 LUMO: 0.19320 factor:1 | 1 (-0.73827) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.54224 HOMO: -7.24095 LUMO: 0.33470 factor:1 | 1 (-0.62439) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.95695 HOMO: -7.15932 LUMO: -2.24222 factor:1 | 1 (-0.03910) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80823 HOMO: -6.88992 LUMO: -2.69937 factor:1 | 1 (-0.89038) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.24216 HOMO: -6.97428 LUMO: -0.98233 factor:1 | 1 (-0.32431) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.97998 HOMO: -7.17564 LUMO: -0.93879 factor:1 | 1 (-2.06213) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17336 HOMO: -6.81645 LUMO: -1.14288 factor:1 | 1 (-1.25551) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.98513 HOMO: -6.83006 LUMO: -0.63403 factor:1 | 1 (-2.06728) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01308 HOMO: -7.17292 LUMO: -1.07213 factor:1 | 1 (-1.09523) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23692 HOMO: -7.53755 LUMO: 0.15510 factor:1 | 1 (-1.31907) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.04978 HOMO: -6.50080 LUMO: -0.51702 factor:1 | 1 (-2.13193) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.55709 HOMO: -6.72665 LUMO: -0.80001 factor:1 | 1 (-1.63924) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91942 HOMO: -6.72665 LUMO: 1.68711 factor:1 | 1 (-1.00157) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.10855 HOMO: -7.11850 LUMO: -0.75103 factor:1 | 1 (-0.19070) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.02729 HOMO: -6.87087 LUMO: -0.85988 factor:1 | 1 (-1.10944) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.94466 HOMO: -7.08857 LUMO: -0.89798 factor:1 | 1 (-2.02681) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.56419 HOMO: -6.71305 LUMO: -0.85444 factor:1 | 1 (-1.64634) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.97931 HOMO: -6.59332 LUMO: -0.60137 factor:1 | 1 (-1.06146) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.94088 HOMO: -7.28993 LUMO: 0.03265 factor:1 | 1 (-2.02303) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.57943 HOMO: -7.32258 LUMO: 0.13878 factor:1 | 1 (-1.66158) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.94750 HOMO: -7.28993 LUMO: 0.11429 factor:1 | 1 (-1.02965) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.60166 HOMO: -6.86271 LUMO: -1.03947 factor:1 | 1 (-1.68381) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.09284 HOMO: -6.55794 LUMO: -0.84900 factor:1 | 1 (-1.17499) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.95866 HOMO: -7.03686 LUMO: 0.11429 factor:1 | 1 (-1.04081) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.24833 HOMO: -7.06952 LUMO: -0.96056 factor:1 | 1 (-0.33048) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87479 HOMO: -6.90897 LUMO: -0.99866 factor:1 | 1 (-0.95694) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.67055 HOMO: -7.00693 LUMO: -0.83539 factor:1 | -1 (0.24730) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.05802 HOMO: -6.74298 LUMO: -0.85172 factor:1 | 1 (-0.14017) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.87593 HOMO: -6.83822 LUMO: -1.07213 factor:1 | -1 (1.04192) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01156 HOMO: -7.21918 LUMO: -1.55377 factor:1 | 1 (-1.09371) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.65708 HOMO: -6.84094 LUMO: -1.09934 factor:1 | -1 (0.26077) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.84233 HOMO: -7.09129 LUMO: -0.85988 factor:1 | 1 (-0.92448) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.79991 HOMO: -6.57971 LUMO: -2.27215 factor:1 | 1 (-0.88206) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91145 HOMO: -6.81373 LUMO: -1.86942 factor:1 | 1 (-0.99360) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.07205 HOMO: -6.59060 LUMO: -2.30480 factor:1 | 1 (-1.15420) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.12973 HOMO: -6.72938 LUMO: -1.23540 factor:1 | -1 (0.78812) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.81083 HOMO: -6.94707 LUMO: -2.62318 factor:1 | -1 (0.10702) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68695 HOMO: -7.28177 LUMO: -0.09796 factor:1 | 1 (-0.76910) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.43514 HOMO: -6.80013 LUMO: -0.79729 factor:1 | 1 (-0.51729) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68140 HOMO: -7.26544 LUMO: 0.12789 factor:1 | 1 (-0.76355) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.29108 HOMO: -6.51713 LUMO: -0.49253 factor:1 | 1 (-0.37323) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.90838 HOMO: -6.68856 LUMO: -0.77280 factor:1 | -1 (0.00947) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.66348 HOMO: -6.41100 LUMO: -0.70750 factor:1 | -1 (0.25437) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.84064 HOMO: -7.56204 LUMO: 0.22041 factor:1 | 1 (-0.92279) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80921 HOMO: -6.68312 LUMO: 1.30343 factor:1 | 1 (-0.89136) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.10993 HOMO: -7.24367 LUMO: 0.17415 factor:1 | 1 (-1.19208) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.86388 HOMO: -7.52395 LUMO: 1.16737 factor:1 | 1 (-0.94603) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.14634 HOMO: -6.89264 LUMO: 0.23130 factor:1 | 1 (-0.22849) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45576 HOMO: -7.21102 LUMO: 0.19048 factor:1 | 1 (-0.53791) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.52639 HOMO: -7.08312 LUMO: 0.25034 factor:1 | -1 (0.39146) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.61840 HOMO: -6.49536 LUMO: -0.65852 factor:1 | -1 (1.29945) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87890 HOMO: -6.85455 LUMO: 0.13606 factor:1 | 1 (-0.96105) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.86932 HOMO: -7.10217 LUMO: 0.35919 factor:1 | 1 (-0.95147) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64967 HOMO: -7.77429 LUMO: 1.19186 factor:1 | 1 (-0.73182) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59413 HOMO: -6.57427 LUMO: -0.50069 factor:1 | 1 (-0.67628) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60826 HOMO: -7.36340 LUMO: 0.10068 factor:1 | 1 (-0.69041) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.61672 HOMO: -7.28177 LUMO: 0.15238 factor:1 | 1 (-0.69887) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.78384 HOMO: -6.86543 LUMO: -0.84355 factor:1 | 1 (-1.86599) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.33698 HOMO: -6.55794 LUMO: 1.39594 factor:1 | 1 (-1.41913) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62967 HOMO: -6.26134 LUMO: 1.53744 factor:1 | 1 (-0.71182) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20190 HOMO: -5.97562 LUMO: 1.42316 factor:1 | 1 (-1.28405) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36838 HOMO: -6.65046 LUMO: 1.44492 factor:1 | 1 (-1.45053) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.57002 HOMO: -6.92258 LUMO: 0.17415 factor:1 | 1 (-1.65217) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.86293 HOMO: -7.40966 LUMO: 0.19592 factor:1 | 1 (-0.94508) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70861 HOMO: -7.17564 LUMO: 0.16871 factor:1 | 1 (-0.79076) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30277 HOMO: -7.46953 LUMO: 0.22313 factor:1 | 1 (-1.38492) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50645 HOMO: -6.13345 LUMO: 1.85854 factor:1 | 1 (-1.58860) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45898 HOMO: -6.99333 LUMO: -1.65717 factor:1 | 1 (-0.54113) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46330 HOMO: -6.93074 LUMO: -1.79323 factor:1 | 1 (-0.54545) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.35614 HOMO: -6.87904 LUMO: -1.79323 factor:1 | 1 (-1.43829) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.72251 HOMO: -6.84094 LUMO: 0.66940 factor:1 | 1 (-1.80466) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52050 HOMO: -7.13210 LUMO: -1.17553 factor:1 | 1 (-0.60265) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68597 HOMO: -6.52801 LUMO: -2.23678 factor:1 | 1 (-0.76812) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11665 HOMO: -6.81917 LUMO: -1.86398 factor:1 | 1 (-1.19880) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.71686 HOMO: -7.30626 LUMO: -1.66806 factor:1 | 1 (-0.79901) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70184 HOMO: -6.98516 LUMO: -1.40683 factor:1 | 1 (-0.78399) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.84173 HOMO: -6.95523 LUMO: -0.97145 factor:1 | 1 (-0.92388) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.77983 HOMO: -6.83278 LUMO: -2.68848 factor:1 | -1 (0.13802) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.47857 HOMO: -7.25456 LUMO: -2.97420 factor:1 | 1 (-0.56072) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62608 HOMO: -6.80557 LUMO: -2.65039 factor:1 | 1 (-0.70823) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.39519 HOMO: -7.10489 LUMO: 0.77008 factor:1 | 1 (-0.47734) | 1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77719 HOMO: -7.28993 LUMO: -1.06124 factor:1 | 1 (-0.85934) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.75977 HOMO: -7.11578 LUMO: -1.10206 factor:1 | 1 (-0.84192) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.40375 HOMO: -6.91713 LUMO: -1.36329 factor:1 | -1 (1.51410) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89444 HOMO: -7.07224 LUMO: 0.51974 factor:1 | 1 (-0.97659) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76758 HOMO: -7.22734 LUMO: -0.93335 factor:1 | 1 (-0.84973) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.66015 HOMO: -7.19469 LUMO: -0.96600 factor:1 | 1 (-0.74230) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45710 HOMO: -6.93890 LUMO: -0.66940 factor:1 | 1 (-0.53925) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.61768 HOMO: -7.09673 LUMO: -1.05852 factor:1 | -1 (0.30017) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.86847 HOMO: -7.19197 LUMO: -2.26943 factor:1 | 1 (-1.95062) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91063 HOMO: -6.90081 LUMO: -2.64767 factor:1 | 1 (-0.99278) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.12857 HOMO: -6.93890 LUMO: -2.65039 factor:1 | 1 (-1.21072) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46262 HOMO: -6.80013 LUMO: -2.54154 factor:1 | 1 (-0.54477) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77700 HOMO: -6.68040 LUMO: -0.89798 factor:1 | 1 (-0.85915) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.92074 HOMO: -7.01782 LUMO: -1.09662 factor:1 | 1 (-2.00289) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.90108 HOMO: -6.58516 LUMO: -0.83539 factor:1 | 1 (-0.98323) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.85448 HOMO: -7.46953 LUMO: 0.06259 factor:1 | 1 (-1.93663) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17564 HOMO: -6.96884 LUMO: -0.99866 factor:1 | 1 (-1.25779) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50864 HOMO: -7.29809 LUMO: -0.19320 factor:1 | 1 (-0.59079) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.28571 HOMO: -6.86271 LUMO: 0.04082 factor:1 | 1 (-1.36786) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80864 HOMO: -6.36746 LUMO: -1.02587 factor:1 | 1 (-0.89079) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62970 HOMO: -7.15659 LUMO: -1.25989 factor:1 | 1 (-0.71185) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.36270 HOMO: -6.69128 LUMO: -0.59865 factor:1 | 1 (-0.44485) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.38619 HOMO: -7.09129 LUMO: -1.08573 factor:1 | 1 (-0.46834) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89670 HOMO: -6.64502 LUMO: -0.66396 factor:1 | 1 (-0.97885) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.36447 HOMO: -6.93346 LUMO: -0.87349 factor:1 | 1 (-0.44662) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.15551 HOMO: -6.77019 LUMO: -0.87349 factor:1 | 1 (-1.23766) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.43410 HOMO: -6.59060 LUMO: -0.82995 factor:1 | 1 (-0.51625) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.75460 HOMO: -7.17564 LUMO: -1.08846 factor:1 | 1 (-0.83675) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.09850 HOMO: -7.27088 LUMO: -1.18642 factor:1 | 1 (-1.18065) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.34879 HOMO: -7.06680 LUMO: -1.13199 factor:1 | 1 (-1.43094) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52140 HOMO: -7.21918 LUMO: -1.03947 factor:1 | 1 (-0.60355) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.36531 HOMO: -7.26000 LUMO: -0.11973 factor:1 | 1 (-0.44746) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.42842 HOMO: -6.77564 LUMO: 0.23402 factor:1 | 1 (-0.51057) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.52971 HOMO: -7.07224 LUMO: -0.75648 factor:1 | -1 (0.38814) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36887 HOMO: -7.45048 LUMO: 0.18232 factor:1 | 1 (-1.45102) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64121 HOMO: -7.48313 LUMO: 0.15238 factor:1 | 1 (-0.72336) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20963 HOMO: -6.60692 LUMO: -0.50885 factor:1 | 1 (-1.29178) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27998 HOMO: -6.62869 LUMO: -0.60954 factor:1 | 1 (-0.36213) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91847 HOMO: -7.40422 LUMO: -1.28982 factor:1 | 1 (-1.00062) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.77797 HOMO: -6.75114 LUMO: -1.23268 factor:1 | 1 (-1.86012) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.40737 HOMO: -6.84638 LUMO: -0.73199 factor:1 | 1 (-2.48952) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.15749 HOMO: -6.79196 LUMO: -1.43676 factor:1 | 1 (-1.23964) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.62558 HOMO: -7.00965 LUMO: -1.37690 factor:1 | 1 (-1.70773) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.41448 HOMO: -6.97972 LUMO: -1.58098 factor:1 | 1 (-1.49663) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.48097 HOMO: -6.91169 LUMO: -1.48574 factor:1 | 1 (-2.56312) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.84379 HOMO: -6.90081 LUMO: -1.30343 factor:1 | 1 (-1.92594) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.48689 HOMO: -6.78652 LUMO: -1.51840 factor:1 | 1 (-1.56904) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.99975 HOMO: -6.84638 LUMO: -1.15104 factor:1 | 1 (-1.08190) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46333 HOMO: -6.61237 LUMO: -0.89798 factor:1 | 1 (-0.54548) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.91280 HOMO: -7.16204 LUMO: -1.30070 factor:1 | 1 (-1.99495) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11510 HOMO: -7.32803 LUMO: 0.14694 factor:1 | 1 (-1.19725) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.63297 HOMO: -6.99877 LUMO: -0.87621 factor:1 | 1 (-2.71512) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.93868 HOMO: -6.99877 LUMO: -0.97145 factor:1 | 1 (-2.02083) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.52000 HOMO: -7.08040 LUMO: -1.09662 factor:1 | 1 (-1.60215) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.72120 HOMO: -6.90897 LUMO: -1.14016 factor:1 | 1 (-1.80335) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.18657 HOMO: -6.68312 LUMO: -0.74831 factor:1 | 1 (-2.26872) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.55840 HOMO: -6.99061 LUMO: -0.86804 factor:1 | 1 (-1.64055) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.79132 HOMO: -7.10761 LUMO: -1.18642 factor:1 | 1 (-2.87347) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.84552 HOMO: -6.79196 LUMO: -0.71294 factor:1 | 1 (-2.92767) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.38163 HOMO: -6.86271 LUMO: -0.81362 factor:1 | 1 (-1.46378) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.66313 HOMO: -7.01510 LUMO: -0.99322 factor:1 | 1 (-1.74528) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.94981 HOMO: -6.88720 LUMO: -0.87893 factor:1 | 1 (-2.03196) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.21796 HOMO: -6.88448 LUMO: 0.22041 factor:1 | 1 (-1.30011) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.03471 HOMO: -7.55932 LUMO: 1.12111 factor:1 | 1 (-2.11686) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36177 HOMO: -6.46815 LUMO: -0.86260 factor:1 | 1 (-1.44392) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.97749 HOMO: -7.13755 LUMO: 0.23130 factor:1 | 1 (-1.05964) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.08554 HOMO: -6.78924 LUMO: 1.51023 factor:1 | 1 (-2.16769) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.09860 HOMO: -6.48992 LUMO: 1.74969 factor:1 | 1 (-2.18075) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.44950 HOMO: -6.78380 LUMO: 1.81500 factor:1 | 1 (-1.53165) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01771 HOMO: -6.49536 LUMO: 1.70615 factor:1 | 1 (-1.09986) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.48778 HOMO: -6.38651 LUMO: 1.44492 factor:1 | 1 (-2.56992) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.41771 HOMO: -6.83822 LUMO: 1.38234 factor:1 | 1 (-1.49986) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.12744 HOMO: -6.01644 LUMO: 1.20274 factor:1 | 1 (-2.20959) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.29902 HOMO: -6.18243 LUMO: 1.77962 factor:1 | 1 (-1.38117) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.32243 HOMO: -6.81917 LUMO: -1.01771 factor:1 | 1 (-0.40458) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36653 HOMO: -6.61237 LUMO: -0.91702 factor:1 | 1 (-1.44868) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.23562 HOMO: -6.84094 LUMO: -0.84900 factor:1 | 1 (-0.31777) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30226 HOMO: -6.81917 LUMO: -1.01771 factor:1 | 1 (-1.38441) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68350 HOMO: -7.86953 LUMO: 1.16737 factor:1 | 1 (-0.76565) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.73081 HOMO: -7.40694 LUMO: 0.11429 factor:1 | 1 (-1.81296) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64360 HOMO: -6.70489 LUMO: -0.65035 factor:1 | 1 (-0.72575) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.55361 HOMO: -7.23279 LUMO: 0.33470 factor:1 | 1 (-1.63576) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.29576 HOMO: -7.17020 LUMO: 0.41361 factor:1 | 1 (-0.37791) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57313 HOMO: -6.90353 LUMO: -0.90070 factor:1 | 1 (-0.65528) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20402 HOMO: -7.39061 LUMO: 0.17687 factor:1 | 1 (-1.28617) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27168 HOMO: -7.16748 LUMO: 0.42178 factor:1 | 1 (-0.35383) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.41332 HOMO: -7.36884 LUMO: -1.11295 factor:1 | 1 (-0.49546) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.96192 HOMO: -7.33347 LUMO: 0.33198 factor:1 | 1 (-2.04406) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61946 HOMO: -7.31986 LUMO: -0.83539 factor:1 | 1 (-1.70161) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50501 HOMO: -7.31170 LUMO: 0.08708 factor:1 | 1 (-1.58716) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.71266 HOMO: -7.36884 LUMO: 0.38096 factor:1 | 1 (-1.79481) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20000 HOMO: -6.99333 LUMO: 1.74153 factor:1 | 1 (-1.28215) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.15173 HOMO: -6.94435 LUMO: 1.74969 factor:1 | 1 (-0.23388) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.38362 HOMO: -7.02598 LUMO: 1.43404 factor:1 | 1 (-1.46577) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.41356 HOMO: -6.41100 LUMO: 1.62996 factor:1 | 1 (-0.49571) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17902 HOMO: -6.57699 LUMO: 1.81228 factor:1 | 1 (-1.26117) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.55212 HOMO: -6.86543 LUMO: 1.49935 factor:1 | 1 (-0.63427) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64679 HOMO: -6.91169 LUMO: -1.22451 factor:1 | 1 (-0.72894) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.97625 HOMO: -7.09945 LUMO: -1.23812 factor:1 | 1 (-0.05840) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.78108 HOMO: -7.48857 LUMO: 0.10340 factor:1 | 1 (-0.86323) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.83139 HOMO: -7.21918 LUMO: -0.06803 factor:1 | 1 (-0.91354) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.18915 HOMO: -6.34025 LUMO: -0.68845 factor:1 | 1 (-0.27130) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68897 HOMO: -6.82734 LUMO: -0.77825 factor:1 | 1 (-0.77112) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.48445 HOMO: -6.92258 LUMO: -1.03675 factor:1 | 1 (-0.56660) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.82630 HOMO: -6.42461 LUMO: -0.95240 factor:1 | 1 (-0.90845) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85049 HOMO: -6.96067 LUMO: -1.05036 factor:1 | 1 (-0.93264) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60619 HOMO: -7.23551 LUMO: 0.12245 factor:1 | 1 (-0.68834) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.96493 HOMO: -6.85183 LUMO: 0.16055 factor:1 | 1 (-0.04708) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64513 HOMO: -6.46815 LUMO: -0.89253 factor:1 | 1 (-0.72728) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91517 HOMO: -7.23823 LUMO: -0.06259 factor:1 | 1 (-0.99732) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77659 HOMO: -6.76475 LUMO: -0.99049 factor:1 | 1 (-0.85874) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.22588 HOMO: -7.14843 LUMO: -0.88165 factor:1 | 1 (-0.30803) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76018 HOMO: -7.15659 LUMO: 0.20681 factor:1 | 1 (-0.84233) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69691 HOMO: -7.11306 LUMO: 0.14150 factor:1 | 1 (-0.77906) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50779 HOMO: -6.67223 LUMO: -0.86260 factor:1 | 1 (-0.58994) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.78617 HOMO: -6.92530 LUMO: 0.30749 factor:1 | 1 (-0.86832) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85038 HOMO: -6.50624 LUMO: -0.70477 factor:1 | 1 (-0.93253) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.10897 HOMO: -7.35524 LUMO: 0.75103 factor:1 | 1 (-2.19112) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23409 HOMO: -7.07768 LUMO: -0.26939 factor:1 | 1 (-1.31624) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.62047 HOMO: -7.15932 LUMO: 0.42450 factor:1 | 1 (-1.70262) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.74325 HOMO: -7.46136 LUMO: 0.04626 factor:1 | 1 (-0.82540) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.66594 HOMO: -7.05047 LUMO: -1.06669 factor:1 | 1 (-1.74809) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57038 HOMO: -6.66951 LUMO: -0.99322 factor:1 | 1 (-0.65253) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.90790 HOMO: -7.01782 LUMO: -1.08846 factor:1 | 1 (-1.99005) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01553 HOMO: -7.03959 LUMO: -1.15376 factor:1 | 1 (-1.09768) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.80085 HOMO: -6.68856 LUMO: 1.61364 factor:1 | 1 (-1.88300) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80086 HOMO: -6.53345 LUMO: 1.60275 factor:1 | 1 (-0.88301) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50333 HOMO: -6.73482 LUMO: 1.86398 factor:1 | 1 (-0.58548) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.71781 HOMO: -6.87632 LUMO: 1.59731 factor:1 | 1 (-0.79996) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.78820 HOMO: -6.31848 LUMO: 2.12521 factor:1 | 1 (-1.87035) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.29681 HOMO: -6.35114 LUMO: 1.71432 factor:1 | 1 (-1.37896) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50899 HOMO: -6.34842 LUMO: 1.92929 factor:1 | 1 (-0.59114) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.03004 HOMO: -6.14977 LUMO: 1.78235 factor:1 | 1 (-0.11219) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59835 HOMO: -6.31032 LUMO: 1.51567 factor:1 | 1 (-0.68050) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.52210 HOMO: -6.25862 LUMO: 1.75241 factor:1 | 1 (-1.60425) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.37761 HOMO: -6.49264 LUMO: 1.66806 factor:1 | 1 (-0.45976) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.96747 HOMO: -6.28311 LUMO: 1.60003 factor:1 | 1 (-2.04962) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.56051 HOMO: -7.13210 LUMO: -0.04354 factor:1 | 1 (-2.64266) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.41821 HOMO: -7.35252 LUMO: 0.03537 factor:1 | 1 (-0.50036) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.71622 HOMO: -6.58243 LUMO: -0.48980 factor:1 | 1 (-1.79837) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.48064 HOMO: -6.90081 LUMO: -0.05442 factor:1 | -1 (0.43721) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.72281 HOMO: -7.22734 LUMO: 0.17143 factor:1 | 1 (-1.80496) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.93552 HOMO: -7.13210 LUMO: -0.99866 factor:1 | 1 (-2.01767) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64282 HOMO: -7.39878 LUMO: 0.13334 factor:1 | 1 (-0.72497) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60178 HOMO: -7.04503 LUMO: -0.89798 factor:1 | 1 (-0.68393) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62126 HOMO: -6.95523 LUMO: -1.07213 factor:1 | 1 (-0.70341) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.51776 HOMO: -6.75114 LUMO: -1.28438 factor:1 | 1 (-2.59991) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61864 HOMO: -6.75114 LUMO: -0.11701 factor:1 | 1 (-1.70079) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.21066 HOMO: -6.83278 LUMO: -0.01633 factor:1 | 1 (-1.29281) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.67475 HOMO: -6.93890 LUMO: -0.88981 factor:1 | 1 (-1.75690) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.24073 HOMO: -7.07224 LUMO: -1.08573 factor:1 | 1 (-1.32288) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.85606 HOMO: -6.99877 LUMO: -0.95240 factor:1 | 1 (-1.93821) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.44547 HOMO: -7.09129 LUMO: 0.35375 factor:1 | 1 (-1.52762) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.64594 HOMO: -7.09401 LUMO: 0.04354 factor:1 | 1 (-1.72809) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.26122 HOMO: -6.85183 LUMO: -0.68573 factor:1 | 1 (-1.34337) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.43488 HOMO: -6.83006 LUMO: -0.58777 factor:1 | 1 (-1.51703) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45326 HOMO: -7.40422 LUMO: 0.17687 factor:1 | 1 (-0.53541) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27641 HOMO: -7.15932 LUMO: 0.10340 factor:1 | 1 (-0.35856) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70116 HOMO: -7.03414 LUMO: -0.19592 factor:1 | 1 (-0.78331) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59963 HOMO: -6.48447 LUMO: -0.36191 factor:1 | 1 (-0.68178) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59068 HOMO: -7.49402 LUMO: 0.11429 factor:1 | 1 (-0.67283) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.92835 HOMO: -7.01237 LUMO: -1.06397 factor:1 | 1 (-0.01050) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.65019 HOMO: -6.67223 LUMO: -1.07213 factor:1 | 1 (-0.73234) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89858 HOMO: -7.38789 LUMO: -1.15376 factor:1 | 1 (-0.98073) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.44415 HOMO: -6.42461 LUMO: -1.23812 factor:1 | 1 (-0.52630) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.33788 HOMO: -7.36884 LUMO: -1.19186 factor:1 | 1 (-1.42003) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.51021 HOMO: -6.65591 LUMO: 0.07075 factor:1 | 1 (-0.59236) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.22642 HOMO: -7.39061 LUMO: -0.16871 factor:1 | 1 (-1.30857) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.72404 HOMO: -6.90353 LUMO: -0.96056 factor:1 | 1 (-0.80619) | -1 | -1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50015 HOMO: -7.42054 LUMO: 0.19048 factor:1 | 1 (-0.58230) | 1 | 1 |
| G: -6694.55216 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.26107 HOMO: -7.40150 LUMO: 0.35647 factor:1 | 1 (-0.34322) | 1 | 1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12855.83922 HOMO: -6.56067 LUMO: -0.96056 factor:1 | 1 (-0.23600) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12853.73390 HOMO: -6.89809 LUMO: -0.81090 factor:1 | -1 (1.86931) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.66477 HOMO: -6.91986 LUMO: -0.84900 factor:1 | -1 (0.93844) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.39198 HOMO: -6.61509 LUMO: -0.62042 factor:1 | -1 (1.21123) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.41799 HOMO: -6.58243 LUMO: -0.65579 factor:1 | -1 (1.18522) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.70047 HOMO: -6.52257 LUMO: -0.92519 factor:1 | -1 (0.90274) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.36553 HOMO: -6.69128 LUMO: 1.49118 factor:1 | -1 (1.23768) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.36545 HOMO: -7.02870 LUMO: 1.67894 factor:1 | -1 (1.23776) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12852.72038 HOMO: -6.88720 LUMO: 1.68711 factor:1 | -1 (2.88283) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.16354 HOMO: -5.89943 LUMO: 1.03675 factor:1 | -1 (1.43967) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.18079 HOMO: -6.40556 LUMO: 1.14560 factor:1 | 1 (-1.57758) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.78948 HOMO: -6.51168 LUMO: 1.48030 factor:1 | 1 (-2.18627) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.16841 HOMO: -6.64502 LUMO: 1.91568 factor:1 | 1 (-1.56520) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.09342 HOMO: -6.47903 LUMO: 1.91296 factor:1 | 1 (-0.49021) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.16800 HOMO: -6.34297 LUMO: 1.91840 factor:1 | 1 (-1.56479) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.86214 HOMO: -6.89809 LUMO: 1.82861 factor:1 | 1 (-2.25893) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.22071 HOMO: -6.10079 LUMO: 1.62996 factor:1 | 1 (-1.61750) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.53851 HOMO: -7.16476 LUMO: -0.92247 factor:1 | 1 (-1.93530) | 1 | 1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.69520 HOMO: -7.10489 LUMO: -0.95784 factor:1 | 1 (-1.09199) | 1 | 1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.36349 HOMO: -6.76475 LUMO: -0.99866 factor:1 | 1 (-1.76028) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.12680 HOMO: -6.81373 LUMO: -1.05036 factor:1 | 1 (-1.52359) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.14811 HOMO: -6.90081 LUMO: -1.03947 factor:1 | 1 (-1.54490) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.54357 HOMO: -7.06952 LUMO: -0.91702 factor:1 | 1 (-1.94036) | 1 | 1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.22376 HOMO: -6.73482 LUMO: -0.94151 factor:1 | 1 (-1.62055) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.22389 HOMO: -6.99605 LUMO: -1.04764 factor:1 | 1 (-1.62068) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12858.00745 HOMO: -7.03686 LUMO: -0.93335 factor:1 | 1 (-2.40423) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.70388 HOMO: -6.81101 LUMO: -0.95240 factor:1 | 1 (-2.10066) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.95956 HOMO: -6.83822 LUMO: -0.65307 factor:1 | 1 (-1.35635) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.92743 HOMO: -7.05319 LUMO: -0.81634 factor:1 | 1 (-1.32421) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.63302 HOMO: -7.57565 LUMO: 0.19048 factor:1 | 1 (-2.02981) | 1 | 1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12855.88332 HOMO: -6.56067 LUMO: -0.50613 factor:1 | 1 (-0.28011) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.74954 HOMO: -6.74298 LUMO: -0.70477 factor:1 | 1 (-1.14633) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.54836 HOMO: -7.02054 LUMO: 0.03537 factor:1 | -1 (1.05485) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.86111 HOMO: -7.33347 LUMO: -0.17960 factor:1 | 1 (-1.25790) | 1 | 1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.99948 HOMO: -6.98244 LUMO: -0.88165 factor:1 | 1 (-1.39627) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.96617 HOMO: -7.14843 LUMO: -1.19730 factor:1 | 1 (-1.36296) | 1 | 1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.74952 HOMO: -7.17564 LUMO: -1.21907 factor:1 | 1 (-1.14631) | 1 | 1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.67528 HOMO: -6.74026 LUMO: -0.86532 factor:1 | 1 (-1.07207) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.82832 HOMO: -6.82462 LUMO: -1.24084 factor:1 | 1 (-1.22511) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.54352 HOMO: -6.78924 LUMO: -0.70477 factor:1 | 1 (-1.94031) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.86119 HOMO: -7.41238 LUMO: 0.05987 factor:1 | 1 (-1.25798) | 1 | 1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.29984 HOMO: -6.75931 LUMO: 0.02721 factor:1 | 1 (-1.69663) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12858.03749 HOMO: -6.28583 LUMO: -0.93063 factor:1 | 1 (-2.43428) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.94130 HOMO: -6.69128 LUMO: -0.83539 factor:1 | 1 (-1.33809) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.09497 HOMO: -7.22190 LUMO: 0.01361 factor:1 | 1 (-1.49176) | 1 | 1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.81768 HOMO: -6.95251 LUMO: -1.09934 factor:1 | 1 (-1.21447) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.24558 HOMO: -6.75387 LUMO: -0.90614 factor:1 | 1 (-1.64237) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.88383 HOMO: -7.48585 LUMO: 0.05987 factor:1 | 1 (-1.28062) | 1 | 1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.75444 HOMO: -6.92802 LUMO: -0.66940 factor:1 | 1 (-1.15123) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.74796 HOMO: -7.29537 LUMO: -0.14150 factor:1 | 1 (-2.14475) | 1 | 1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12858.18922 HOMO: -6.57155 LUMO: -0.86804 factor:1 | 1 (-2.58601) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12855.87761 HOMO: -6.87632 LUMO: -0.77825 factor:1 | 1 (-0.27440) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.22505 HOMO: -6.45998 LUMO: -0.31565 factor:1 | 1 (-0.62183) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.86571 HOMO: -7.51306 LUMO: 0.05714 factor:1 | 1 (-1.26250) | 1 | 1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12855.67287 HOMO: -6.86271 LUMO: -0.00816 factor:1 | 1 (-0.06966) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.86264 HOMO: -6.43277 LUMO: -1.07485 factor:1 | 1 (-1.25942) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.24411 HOMO: -6.78108 LUMO: -0.81362 factor:1 | 1 (-1.64090) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.96604 HOMO: -6.88448 LUMO: 1.21907 factor:1 | 1 (-1.36283) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.80276 HOMO: -6.97700 LUMO: 1.44765 factor:1 | 1 (-2.19955) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.77408 HOMO: -6.89537 LUMO: 2.12249 factor:1 | 1 (-2.17087) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.85259 HOMO: -6.28311 LUMO: 1.45037 factor:1 | 1 (-1.24938) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12858.17948 HOMO: -6.55522 LUMO: 1.39867 factor:1 | 1 (-2.57627) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.05241 HOMO: -6.46815 LUMO: 1.50207 factor:1 | 1 (-1.44920) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.54371 HOMO: -6.43549 LUMO: 2.17419 factor:1 | 1 (-1.94050) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.96590 HOMO: -6.99333 LUMO: 1.87214 factor:1 | 1 (-1.36269) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.91249 HOMO: -6.65591 LUMO: 1.37962 factor:1 | 1 (-1.30928) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.77472 HOMO: -6.82734 LUMO: 1.55649 factor:1 | 1 (-1.17150) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.85270 HOMO: -6.71849 LUMO: 1.36057 factor:1 | 1 (-1.24949) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.94767 HOMO: -6.79468 LUMO: 1.82044 factor:1 | 1 (-1.34446) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.65618 HOMO: -6.61237 LUMO: 1.15104 factor:1 | 1 (-1.05297) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.83484 HOMO: -6.62053 LUMO: 2.33474 factor:1 | 1 (-2.23163) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.10582 HOMO: -6.55794 LUMO: 1.65717 factor:1 | 1 (-1.50261) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.53454 HOMO: -6.85999 LUMO: 2.03813 factor:1 | 1 (-1.93133) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.47286 HOMO: -6.45726 LUMO: 1.28438 factor:1 | 1 (-0.86965) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.72046 HOMO: -6.23685 LUMO: 1.93201 factor:1 | 1 (-1.11725) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.88035 HOMO: -7.06680 LUMO: 1.86942 factor:1 | 1 (-1.27714) | 1 | 1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.12253 HOMO: -6.89537 LUMO: 2.17147 factor:1 | 1 (-1.51932) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.38374 HOMO: -6.80013 LUMO: 1.78779 factor:1 | 1 (-0.78053) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.86416 HOMO: -6.45726 LUMO: 1.58370 factor:1 | 1 (-1.26095) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.87570 HOMO: -6.52529 LUMO: 1.71976 factor:1 | 1 (-1.27249) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.85967 HOMO: -7.22462 LUMO: -1.18642 factor:1 | 1 (-1.25646) | 1 | 1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.69861 HOMO: -7.18381 LUMO: -0.78641 factor:1 | 1 (-1.09539) | 1 | 1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.84693 HOMO: -6.93346 LUMO: 1.65717 factor:1 | 1 (-1.24372) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.84334 HOMO: -6.41644 LUMO: 1.78235 factor:1 | 1 (-1.24013) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.79493 HOMO: -6.59876 LUMO: 1.83677 factor:1 | 1 (-1.19172) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.53098 HOMO: -6.35658 LUMO: 1.59731 factor:1 | 1 (-0.92777) | -1 | -1 |
| G: -6591.23752 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.82557 HOMO: -6.60692 LUMO: 1.66534 factor:1 | 1 (-1.22236) | -1 | -1 |
| G: -6590.76945 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12855.83922 HOMO: -6.83006 LUMO: 2.11705 factor:1 | 1 (-0.70407) | -1 | -1 |
| G: -6590.76945 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12853.73390 HOMO: -6.89264 LUMO: 1.30070 factor:1 | -1 (1.40125) | -1 | -1 |
| G: -6590.76945 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.66477 HOMO: -6.90081 LUMO: 2.05174 factor:1 | -1 (0.47038) | -1 | -1 |
| G: -6590.76945 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.39198 HOMO: -6.74842 LUMO: 1.96194 factor:1 | -1 (0.74317) | -1 | -1 |
| G: -6590.76945 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.41799 HOMO: -6.58516 LUMO: 1.30887 factor:1 | -1 (0.71716) | -1 | -1 |
| G: -6590.76945 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.70047 HOMO: -7.00965 LUMO: 2.08167 factor:1 | -1 (0.43467) | -1 | -1 |
| G: -6590.76945 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.36553 HOMO: -6.86815 LUMO: 2.29664 factor:1 | -1 (0.76962) | -1 | -1 |
| G: -6590.76945 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.36545 HOMO: -6.39740 LUMO: 2.02725 factor:1 | -1 (0.76970) | -1 | -1 |
| G: -6590.76945 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12852.72038 HOMO: -5.95929 LUMO: 1.62724 factor:1 | -1 (2.41477) | -1 | -1 |
| G: -6590.76945 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.16354 HOMO: -6.71849 LUMO: 1.34696 factor:1 | -1 (0.97161) | -1 | -1 |
| G: -6590.76945 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.18079 HOMO: -7.26816 LUMO: 1.74153 factor:1 | 1 (-2.04564) | 1 | 1 |
| G: -6590.76945 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.78948 HOMO: -6.90897 LUMO: 1.71432 factor:1 | 1 (-2.65433) | -1 | -1 |
| G: -6590.76945 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.16841 HOMO: -6.70489 LUMO: 1.91568 factor:1 | 1 (-2.03326) | -1 | -1 |
| G: -6590.76945 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.09342 HOMO: -6.83278 LUMO: 1.61908 factor:1 | 1 (-0.95828) | -1 | -1 |
| G: -6590.76945 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.16800 HOMO: -7.17292 LUMO: 1.95378 factor:1 | 1 (-2.03285) | 1 | -1 |
| G: -6590.76945 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.86214 HOMO: -6.53345 LUMO: 1.74153 factor:1 | 1 (-2.72699) | -1 | -1 |
| G: -6590.76945 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.22071 HOMO: -6.53073 LUMO: 1.51023 factor:1 | 1 (-2.08556) | -1 | -1 |
| G: -6590.76945 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.53851 HOMO: -6.93346 LUMO: 2.22861 factor:1 | 1 (-2.40336) | -1 | -1 |
| G: -6590.76945 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.69520 HOMO: -6.47903 LUMO: 2.05446 factor:1 | 1 (-1.56006) | -1 | -1 |
| G: -6590.76945 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.36349 HOMO: -6.88992 LUMO: 1.57010 factor:1 | 1 (-2.22834) | -1 | -1 |
| G: -6590.76945 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.12680 HOMO: -6.07358 LUMO: 1.95922 factor:1 | 1 (-1.99166) | -1 | -1 |
| G: -6590.76945 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.14811 HOMO: -6.75114 LUMO: 2.18780 factor:1 | 1 (-2.01296) | -1 | -1 |
| G: -6590.76945 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.54357 HOMO: -6.96339 LUMO: 1.70071 factor:1 | 1 (-2.40843) | -1 | -1 |
| G: -6590.76945 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.22376 HOMO: -7.14843 LUMO: 1.82588 factor:1 | 1 (-2.08861) | 1 | -1 |
| G: -6590.76945 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.22389 HOMO: -6.96339 LUMO: 2.29392 factor:1 | 1 (-2.08875) | -1 | -1 |
| G: -6590.76945 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12858.00745 HOMO: -6.81645 LUMO: 2.39732 factor:1 | 1 (-2.87230) | -1 | -1 |
| G: -6590.76945 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.70388 HOMO: -6.48447 LUMO: 1.24084 factor:1 | 1 (-2.56873) | -1 | -1 |
| G: -6590.76945 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.95956 HOMO: -7.14843 LUMO: 2.01092 factor:1 | 1 (-1.82441) | 1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.92743 HOMO: -7.20013 LUMO: -0.34286 factor:1 | 1 (-1.79228) | 1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.63302 HOMO: -6.97700 LUMO: -0.15238 factor:1 | 1 (-2.49787) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12855.88332 HOMO: -7.07768 LUMO: -0.26123 factor:1 | 1 (-0.74818) | 1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.74954 HOMO: -6.99333 LUMO: -0.41361 factor:1 | 1 (-1.61440) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.54836 HOMO: -6.84638 LUMO: -0.40273 factor:1 | -1 (0.58679) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.86111 HOMO: -6.83822 LUMO: -0.26939 factor:1 | 1 (-1.72596) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.99948 HOMO: -6.75931 LUMO: -0.93879 factor:1 | 1 (-1.86433) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.96617 HOMO: -6.79468 LUMO: -0.39729 factor:1 | 1 (-1.83103) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.74952 HOMO: -6.93890 LUMO: 0.43266 factor:1 | 1 (-1.61437) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.67528 HOMO: -7.08040 LUMO: -0.85716 factor:1 | 1 (-1.54014) | 1 | 1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.82832 HOMO: -6.70216 LUMO: -1.41499 factor:1 | 1 (-1.69317) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.54352 HOMO: -6.63686 LUMO: -0.52790 factor:1 | 1 (-2.40837) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.86119 HOMO: -6.75114 LUMO: -0.13334 factor:1 | 1 (-1.72605) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.29984 HOMO: -6.94435 LUMO: -0.24490 factor:1 | 1 (-2.16469) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12858.03749 HOMO: -6.74298 LUMO: -0.84627 factor:1 | 1 (-2.90234) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.94130 HOMO: -7.15932 LUMO: 0.22041 factor:1 | 1 (-1.80616) | 1 | 1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.09497 HOMO: -6.90081 LUMO: -1.16737 factor:1 | 1 (-1.95982) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.81768 HOMO: -7.04775 LUMO: -0.84355 factor:1 | 1 (-1.68253) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.24558 HOMO: -7.17020 LUMO: -1.31159 factor:1 | 1 (-2.11043) | 1 | 1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.88383 HOMO: -7.14571 LUMO: -0.46259 factor:1 | 1 (-1.74869) | 1 | 1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.75444 HOMO: -7.45048 LUMO: -0.91158 factor:1 | 1 (-1.61930) | 1 | 1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.74796 HOMO: -6.87360 LUMO: -0.82995 factor:1 | 1 (-2.61281) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12858.18922 HOMO: -7.43415 LUMO: -0.65307 factor:1 | 1 (-3.05407) | 1 | 1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12855.87761 HOMO: -7.47225 LUMO: -0.77280 factor:1 | 1 (-0.74246) | 1 | 1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.22505 HOMO: -6.86271 LUMO: -0.83811 factor:1 | 1 (-1.08990) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.86571 HOMO: -7.53483 LUMO: -0.66124 factor:1 | 1 (-1.73056) | 1 | 1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12855.67287 HOMO: -7.45864 LUMO: -1.08301 factor:1 | 1 (-0.53772) | 1 | 1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.86264 HOMO: -7.24639 LUMO: -1.19186 factor:1 | 1 (-1.72749) | 1 | 1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.24411 HOMO: -7.54844 LUMO: -0.96873 factor:1 | 1 (-2.10896) | 1 | 1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.96604 HOMO: -7.12666 LUMO: -0.01633 factor:1 | 1 (-1.83089) | 1 | 1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.80276 HOMO: -6.77291 LUMO: -0.70477 factor:1 | 1 (-2.66761) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.77408 HOMO: -6.76475 LUMO: -1.15921 factor:1 | 1 (-2.63893) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.85259 HOMO: -5.37697 LUMO: -0.56600 factor:1 | 1 (-1.71745) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12858.17948 HOMO: -6.62053 LUMO: -1.75513 factor:1 | 1 (-3.04433) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.05241 HOMO: -6.60420 LUMO: -1.74697 factor:1 | 1 (-1.91726) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.54371 HOMO: -6.84366 LUMO: -0.94968 factor:1 | 1 (-2.40856) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.96590 HOMO: -6.96884 LUMO: -2.11977 factor:1 | 1 (-1.83075) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.91249 HOMO: -6.80829 LUMO: 0.56055 factor:1 | 1 (-1.77734) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.77472 HOMO: -7.02326 LUMO: 0.11429 factor:1 | 1 (-1.63957) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.85270 HOMO: -7.40966 LUMO: 0.18232 factor:1 | 1 (-1.71756) | 1 | 1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.94767 HOMO: -6.34570 LUMO: 0.41089 factor:1 | 1 (-1.81252) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.65618 HOMO: -6.78924 LUMO: 0.49525 factor:1 | 1 (-1.52103) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.83484 HOMO: -6.87632 LUMO: 0.44082 factor:1 | 1 (-2.69970) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.10582 HOMO: -6.69944 LUMO: 1.20546 factor:1 | 1 (-1.97068) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.53454 HOMO: -6.83006 LUMO: 1.28982 factor:1 | 1 (-2.39939) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.47286 HOMO: -7.78246 LUMO: 0.20681 factor:1 | 1 (-1.33771) | 1 | 1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.72046 HOMO: -6.55794 LUMO: -1.65173 factor:1 | 1 (-1.58531) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.88035 HOMO: -6.77564 LUMO: -1.14560 factor:1 | 1 (-1.74520) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.12253 HOMO: -7.46680 LUMO: -1.18097 factor:1 | 1 (-1.98738) | 1 | 1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.38374 HOMO: -6.88176 LUMO: -1.24900 factor:1 | 1 (-1.24859) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.86416 HOMO: -7.28177 LUMO: -0.42178 factor:1 | 1 (-1.72901) | 1 | 1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.87570 HOMO: -7.71715 LUMO: 0.19592 factor:1 | 1 (-1.74055) | 1 | 1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.85967 HOMO: -7.02326 LUMO: -1.40683 factor:1 | 1 (-1.72452) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.69861 HOMO: -7.27088 LUMO: -1.07485 factor:1 | 1 (-1.56346) | 1 | 1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.84693 HOMO: -7.17020 LUMO: -0.49525 factor:1 | 1 (-1.71179) | 1 | 1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.84334 HOMO: -7.15932 LUMO: 0.02721 factor:1 | 1 (-1.70819) | 1 | 1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.79493 HOMO: -7.00693 LUMO: -0.83267 factor:1 | 1 (-1.65979) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.53098 HOMO: -6.86543 LUMO: -0.10340 factor:1 | 1 (-1.39584) | -1 | -1 |
| G: -6590.76945 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.82557 HOMO: -7.11850 LUMO: -0.08980 factor:1 | 1 (-1.69043) | 1 | 1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12855.83922 HOMO: -6.87087 LUMO: -0.88981 factor:1 | 1 (-0.01118) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12853.73390 HOMO: -7.08857 LUMO: -1.27077 factor:1 | -1 (2.09413) | 1 | 1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.66477 HOMO: -6.79468 LUMO: -0.81906 factor:1 | -1 (1.16326) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.39198 HOMO: -6.86815 LUMO: -0.89798 factor:1 | -1 (1.43605) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.41799 HOMO: -6.78652 LUMO: -2.00548 factor:1 | -1 (1.41004) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.70047 HOMO: -6.75114 LUMO: -0.08436 factor:1 | -1 (1.12756) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.36553 HOMO: -6.55794 LUMO: 0.52790 factor:1 | -1 (1.46250) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.36545 HOMO: -7.17836 LUMO: 0.28300 factor:1 | -1 (1.46258) | 1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12852.72038 HOMO: -7.35796 LUMO: -0.77552 factor:1 | -1 (3.10765) | 1 | 1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.16354 HOMO: -7.23551 LUMO: -1.17553 factor:1 | -1 (1.66449) | 1 | 1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.18079 HOMO: -7.07496 LUMO: -1.14288 factor:1 | 1 (-1.35276) | 1 | 1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.78948 HOMO: -6.70489 LUMO: -0.83539 factor:1 | 1 (-1.96145) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.16841 HOMO: -6.59604 LUMO: -0.89798 factor:1 | 1 (-1.34038) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.09342 HOMO: -6.94162 LUMO: -1.22451 factor:1 | 1 (-0.26539) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.16800 HOMO: -6.68040 LUMO: 0.22041 factor:1 | 1 (-1.33997) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.86214 HOMO: -6.88176 LUMO: 0.11157 factor:1 | 1 (-2.03411) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.22071 HOMO: -6.91713 LUMO: 1.27621 factor:1 | 1 (-1.39268) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.53851 HOMO: -6.77836 LUMO: 1.01226 factor:1 | 1 (-1.71048) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.69520 HOMO: -7.14571 LUMO: 1.48574 factor:1 | 1 (-0.86717) | 1 | 1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.36349 HOMO: -6.96884 LUMO: 1.48574 factor:1 | 1 (-1.53546) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.12680 HOMO: -7.24367 LUMO: 1.28438 factor:1 | 1 (-1.29877) | 1 | 1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.14811 HOMO: -7.10489 LUMO: 1.29526 factor:1 | 1 (-1.32008) | 1 | 1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.54357 HOMO: -7.07224 LUMO: 1.29254 factor:1 | 1 (-1.71554) | 1 | 1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.22376 HOMO: -7.12938 LUMO: 0.49253 factor:1 | 1 (-1.39573) | 1 | 1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.22389 HOMO: -7.33619 LUMO: 1.45581 factor:1 | 1 (-1.39586) | 1 | 1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12858.00745 HOMO: -6.87904 LUMO: -0.14422 factor:1 | 1 (-2.17941) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.70388 HOMO: -6.81917 LUMO: 0.50341 factor:1 | 1 (-1.87584) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.95956 HOMO: -7.27905 LUMO: 0.13606 factor:1 | 1 (-1.13153) | 1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.92743 HOMO: -6.87904 LUMO: -0.09796 factor:1 | 1 (-1.09939) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.63302 HOMO: -7.33891 LUMO: 0.03810 factor:1 | 1 (-1.80499) | 1 | 1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12855.88332 HOMO: -6.98516 LUMO: 0.98233 factor:1 | 1 (-0.05529) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.74954 HOMO: -6.94162 LUMO: 0.86804 factor:1 | 1 (-0.92151) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.54836 HOMO: -7.37701 LUMO: 0.05442 factor:1 | -1 (1.27967) | 1 | 1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.86111 HOMO: -7.04775 LUMO: 0.43266 factor:1 | 1 (-1.03308) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.99948 HOMO: -7.47497 LUMO: 0.31837 factor:1 | 1 (-1.17145) | 1 | 1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.96617 HOMO: -6.62053 LUMO: 0.13061 factor:1 | 1 (-1.13814) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.74952 HOMO: -6.44366 LUMO: -0.04354 factor:1 | 1 (-0.92149) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.67528 HOMO: -6.40284 LUMO: 0.68301 factor:1 | 1 (-0.84725) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.82832 HOMO: -6.73754 LUMO: 0.36735 factor:1 | 1 (-1.00029) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.54352 HOMO: -6.85455 LUMO: 0.23946 factor:1 | 1 (-1.71549) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.86119 HOMO: -6.93346 LUMO: 0.24762 factor:1 | 1 (-1.03316) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.29984 HOMO: -6.85455 LUMO: 0.17687 factor:1 | 1 (-1.47181) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12858.03749 HOMO: -6.62325 LUMO: 0.69933 factor:1 | 1 (-2.20946) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.94130 HOMO: -6.43005 LUMO: 0.50069 factor:1 | 1 (-1.11327) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.09497 HOMO: -6.56883 LUMO: 0.22858 factor:1 | 1 (-1.26693) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.81768 HOMO: -6.78380 LUMO: 0.54967 factor:1 | 1 (-0.98965) | -1 | -1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.24558 HOMO: -7.35524 LUMO: 0.00272 factor:1 | 1 (-1.41755) | 1 | 1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.88383 HOMO: -7.27360 LUMO: 0.08436 factor:1 | 1 (-1.05580) | 1 | 1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.75444 HOMO: -7.44504 LUMO: -0.96056 factor:1 | 1 (-0.92641) | 1 | 1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.74796 HOMO: -7.27360 LUMO: 0.29933 factor:1 | 1 (-1.91993) | 1 | 1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12858.18922 HOMO: -7.09129 LUMO: 0.41089 factor:1 | 1 (-2.36119) | 1 | 1 |
| G: -6591.46234 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12855.87761 HOMO: -6.93618 LUMO: 0.36463 factor:1 | 1 (-0.04958) | -1 | -1 |
| G: -6591.46234 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.22505 HOMO: -7.65728 LUMO: 0.20136 factor:1 | 1 (-0.39701) | 1 | 1 |
| G: -6591.46234 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.86571 HOMO: -6.90353 LUMO: -0.92791 factor:1 | 1 (-1.03768) | -1 | -1 |
| G: -6591.46234 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12855.67287 HOMO: -6.82462 LUMO: -1.18370 factor:1 | -1 (0.15516) | -1 | -1 |
| G: -6591.46234 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.86264 HOMO: -7.09129 LUMO: -0.13334 factor:1 | 1 (-1.03460) | 1 | 1 |
| G: -6591.46234 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.24411 HOMO: -7.40966 LUMO: -1.06941 factor:1 | 1 (-1.41608) | 1 | 1 |
| G: -6591.46234 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.96604 HOMO: -7.24367 LUMO: -1.00954 factor:1 | 1 (-1.13801) | 1 | 1 |
| G: -6591.46234 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.80276 HOMO: -7.51851 LUMO: 0.09796 factor:1 | 1 (-1.97473) | 1 | 1 |
| G: -6591.46234 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.77408 HOMO: -7.48857 LUMO: -0.07619 factor:1 | 1 (-1.94605) | 1 | 1 |
| G: -6591.46234 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.85259 HOMO: -6.53345 LUMO: 1.09390 factor:1 | 1 (-1.02456) | -1 | -1 |
| G: -6591.46234 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12858.17948 HOMO: -7.21918 LUMO: 0.08436 factor:1 | 1 (-2.35144) | 1 | 1 |
| G: -6591.46234 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.05241 HOMO: -7.38789 LUMO: 1.02587 factor:1 | 1 (-1.22438) | 1 | -1 |
| G: -6591.46234 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.54371 HOMO: -6.83550 LUMO: -0.67484 factor:1 | 1 (-1.71568) | -1 | -1 |
| G: -6591.46234 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.96590 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-1.13787) | -1 | -1 |
| G: -6591.46234 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.91249 HOMO: -6.79740 LUMO: 1.91296 factor:1 | 1 (-1.08446) | 1 | 1 |
| G: -6591.46234 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.77472 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-0.94668) | -1 | -1 |
| G: -6591.46234 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.85270 HOMO: -6.62597 LUMO: -0.44082 factor:1 | 1 (-1.02467) | -1 | -1 |
| G: -6591.46234 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.94767 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-1.11964) | -1 | -1 |
| G: -6591.46234 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.65618 HOMO: -6.51168 LUMO: -0.23130 factor:1 | 1 (-0.82815) | -1 | -1 |
| G: -6591.46234 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.83484 HOMO: -7.14027 LUMO: 0.49797 factor:1 | 1 (-2.00681) | -1 | -1 |
| G: -6591.46234 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.10582 HOMO: -7.55660 LUMO: 0.24762 factor:1 | 1 (-1.27779) | -1 | -1 |
| G: -6591.46234 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.53454 HOMO: -6.88992 LUMO: -0.64763 factor:1 | 1 (-1.70651) | -1 | -1 |
| G: -6591.46234 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.47286 HOMO: -6.72665 LUMO: -0.45987 factor:1 | 1 (-0.64483) | -1 | -1 |
| G: -6591.46234 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.72046 HOMO: -6.72121 LUMO: -0.58232 factor:1 | 1 (-0.89242) | -1 | -1 |
| G: -6591.46234 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.88035 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-1.05232) | -1 | -1 |
| G: -6591.46234 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.12253 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-1.29450) | -1 | -1 |
| G: -6591.46234 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.38374 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-0.55571) | -1 | -1 |
| G: -6591.46234 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.86416 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-1.03613) | -1 | -1 |
| G: -6591.46234 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.87570 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-1.04767) | -1 | -1 |
| G: -6591.46234 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.85967 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-1.03164) | -1 | -1 |
| G: -6591.46234 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.69861 HOMO: -6.79740 LUMO: -0.55511 factor:1 | 1 (-0.87057) | -1 | -1 |
| G: -6591.46234 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.84693 HOMO: -6.79740 LUMO: -0.67756 factor:1 | 1 (-1.01890) | -1 | -1 |
| G: -6591.46234 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.84334 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-1.01531) | -1 | -1 |
| G: -6591.46234 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.79493 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-0.96690) | -1 | -1 |
| G: -6591.46234 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.53098 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-0.70295) | -1 | -1 |
| G: -6591.46234 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.82557 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-0.99754) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12855.83922 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-0.26264) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12853.73390 HOMO: -6.59332 LUMO: -0.27211 factor:1 | -1 (1.84267) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.66477 HOMO: -6.57427 LUMO: -0.16871 factor:1 | -1 (0.91180) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.39198 HOMO: -6.71033 LUMO: 1.59187 factor:1 | -1 (1.18459) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.41799 HOMO: -6.72121 LUMO: 2.00004 factor:1 | -1 (1.15858) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.70047 HOMO: -6.61509 LUMO: 1.55921 factor:1 | -1 (0.87610) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.36553 HOMO: -6.55250 LUMO: 1.73064 factor:1 | -1 (1.21104) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.36545 HOMO: -6.66135 LUMO: 2.02181 factor:1 | -1 (1.21112) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12852.72038 HOMO: -6.84911 LUMO: 1.98099 factor:1 | -1 (2.85619) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.16354 HOMO: -6.66679 LUMO: 1.98371 factor:1 | -1 (1.41303) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.18079 HOMO: -6.67495 LUMO: 2.04085 factor:1 | 1 (-1.60422) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.78948 HOMO: -6.89809 LUMO: 1.95106 factor:1 | 1 (-2.21291) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.16841 HOMO: -6.50352 LUMO: 1.88847 factor:1 | 1 (-1.59184) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.09342 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-0.51685) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.16800 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-1.59143) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.86214 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-2.28557) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.22071 HOMO: -6.65591 LUMO: 2.20684 factor:1 | 1 (-1.64414) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.53851 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-1.96194) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.69520 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-1.11863) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.36349 HOMO: -6.53617 LUMO: 1.75241 factor:1 | 1 (-1.78692) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.12680 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-1.55023) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.14811 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-1.57154) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.54357 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-1.96700) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.22376 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-1.64719) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.22389 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-1.64732) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12858.00745 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-2.43087) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.70388 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-2.12730) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.95956 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-1.38299) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.92743 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-1.35085) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.63302 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-2.05645) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12855.88332 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-0.30675) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.74954 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-1.17297) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.54836 HOMO: -6.90897 LUMO: 1.91296 factor:1 | -1 (1.02821) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.86111 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-1.28454) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.99948 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-1.42291) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.96617 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-1.38960) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.74952 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-1.17295) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.67528 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-1.09871) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.82832 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-1.25175) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.54352 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-1.96695) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.86119 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-1.28462) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.29984 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-1.72327) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12858.03749 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-2.46092) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.94130 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-1.36473) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.09497 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-1.51840) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.81768 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-1.24111) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.24558 HOMO: -6.75387 LUMO: 1.72248 factor:1 | 1 (-1.66901) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.88383 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-1.30726) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.75444 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-1.17787) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.74796 HOMO: -6.80557 LUMO: 2.02725 factor:1 | 1 (-2.17139) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12858.18922 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-2.61265) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12855.87761 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-0.30104) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.22505 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-0.64847) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.86571 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-1.28914) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12855.67287 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-0.09630) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.86264 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-1.28606) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.24411 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-1.66754) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.96604 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-1.38947) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.80276 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-2.22619) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.77408 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-2.19751) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.85259 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-1.27602) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12858.17948 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-2.60291) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.05241 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-1.47584) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.54371 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-1.96714) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.96590 HOMO: -6.64230 LUMO: 2.16058 factor:1 | 1 (-1.38933) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.91249 HOMO: -6.58788 LUMO: 2.10616 factor:1 | 1 (-1.33592) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.77472 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-1.19814) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.85270 HOMO: -6.31304 LUMO: 2.31841 factor:1 | 1 (-1.27613) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.94767 HOMO: -6.94979 LUMO: 2.07895 factor:1 | 1 (-1.37110) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.65618 HOMO: -6.88992 LUMO: 2.28031 factor:1 | 1 (-1.07961) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.83484 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-2.25827) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.10582 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-1.52925) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.53454 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-1.95797) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.47286 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-0.89629) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.72046 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-1.14389) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.88035 HOMO: -6.31304 LUMO: 2.18507 factor:1 | 1 (-1.30378) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.12253 HOMO: -6.18243 LUMO: 2.01636 factor:1 | 1 (-1.54596) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.38374 HOMO: -6.99877 LUMO: 2.14970 factor:1 | 1 (-0.80717) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.86416 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-1.28759) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.87570 HOMO: -6.36202 LUMO: 2.17419 factor:1 | 1 (-1.29913) | -1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.85967 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-1.28310) | 1 | -1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.69861 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-1.12203) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.84693 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-1.27036) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.84334 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-1.26677) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.79493 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-1.21836) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.53098 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-0.95441) | 1 | 1 |
| G: -6591.21088 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.82557 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-1.24900) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12855.83922 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-0.54485) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12853.73390 HOMO: -6.71305 LUMO: 1.91840 factor:1 | -1 (1.56046) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.66477 HOMO: -6.44094 LUMO: 1.74425 factor:1 | -1 (0.62959) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.39198 HOMO: -6.51985 LUMO: 1.84221 factor:1 | -1 (0.90238) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.41799 HOMO: -6.63414 LUMO: -0.24762 factor:1 | -1 (0.87637) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.70047 HOMO: -6.60420 LUMO: -0.22585 factor:1 | -1 (0.59389) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.36553 HOMO: -7.19741 LUMO: 0.58232 factor:1 | -1 (0.92883) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.36545 HOMO: -6.77019 LUMO: -0.56872 factor:1 | -1 (0.92892) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12852.72038 HOMO: -7.46136 LUMO: 0.28844 factor:1 | -1 (2.57398) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.16354 HOMO: -6.60420 LUMO: -0.54151 factor:1 | -1 (1.13082) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.18079 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-1.88643) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.78948 HOMO: -6.81645 LUMO: -0.57144 factor:1 | 1 (-2.49512) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.16841 HOMO: -7.48041 LUMO: 0.28572 factor:1 | 1 (-1.87405) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.09342 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-0.79906) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.16800 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-1.87364) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.86214 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-2.56778) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.22071 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-1.92635) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.53851 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-2.24415) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.69520 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-1.40084) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.36349 HOMO: -6.50896 LUMO: -0.25034 factor:1 | 1 (-2.06913) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.12680 HOMO: -7.17564 LUMO: -0.68573 factor:1 | 1 (-1.83244) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.14811 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-1.85375) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.54357 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-2.24921) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.22376 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-1.92940) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.22389 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-1.92953) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12858.00745 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-2.71308) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.70388 HOMO: -6.62325 LUMO: 2.02725 factor:1 | 1 (-2.40951) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.95956 HOMO: -6.63414 LUMO: 1.91296 factor:1 | 1 (-1.66520) | 1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.92743 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-1.63306) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.63302 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-2.33866) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12855.88332 HOMO: -6.61237 LUMO: 2.11432 factor:1 | 1 (-0.58896) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.74954 HOMO: -6.62053 LUMO: 2.09256 factor:1 | 1 (-1.45518) | 1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12854.54836 HOMO: -6.78652 LUMO: 2.13609 factor:1 | -1 (0.74600) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.86111 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-1.56675) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.99948 HOMO: -6.85183 LUMO: 2.12793 factor:1 | 1 (-1.70512) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.96617 HOMO: -6.81101 LUMO: 1.83949 factor:1 | 1 (-1.67181) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.74952 HOMO: -6.98788 LUMO: 2.16058 factor:1 | 1 (-1.45516) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.67528 HOMO: -6.62869 LUMO: 2.00820 factor:1 | 1 (-1.38092) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.82832 HOMO: -6.34025 LUMO: 2.25855 factor:1 | 1 (-1.53396) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.54352 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-2.24916) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.86119 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-1.56683) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.29984 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-2.00548) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12858.03749 HOMO: -6.83278 LUMO: 1.53744 factor:1 | 1 (-2.74313) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.94130 HOMO: -6.41917 LUMO: 1.82316 factor:1 | 1 (-1.64694) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.09497 HOMO: -6.56339 LUMO: 1.63813 factor:1 | 1 (-1.80060) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.81768 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-1.52332) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.24558 HOMO: -6.63141 LUMO: 1.92112 factor:1 | 1 (-1.95122) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.88383 HOMO: -6.83822 LUMO: 1.88847 factor:1 | 1 (-1.58947) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.75444 HOMO: -6.84638 LUMO: 1.90480 factor:1 | 1 (-1.46008) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.74796 HOMO: -6.82462 LUMO: 1.70888 factor:1 | 1 (-2.45360) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12858.18922 HOMO: -6.82734 LUMO: 2.12521 factor:1 | 1 (-2.89486) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12855.87761 HOMO: -6.94435 LUMO: 1.87214 factor:1 | 1 (-0.58325) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.22505 HOMO: -6.98516 LUMO: 2.51433 factor:1 | 1 (-0.93068) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.86571 HOMO: -6.74026 LUMO: 2.15514 factor:1 | 1 (-1.57135) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12855.67287 HOMO: -6.93618 LUMO: 2.54426 factor:1 | 1 (-0.37851) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.86264 HOMO: -6.28583 LUMO: 2.53610 factor:1 | 1 (-1.56827) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.24411 HOMO: -6.56883 LUMO: 1.94834 factor:1 | 1 (-1.94975) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.96604 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-1.67168) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.80276 HOMO: -6.19059 LUMO: 1.99732 factor:1 | 1 (-2.50840) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.77408 HOMO: -6.78108 LUMO: 2.03813 factor:1 | 1 (-2.47972) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.85259 HOMO: -6.82189 LUMO: 1.77418 factor:1 | 1 (-1.55823) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12858.17948 HOMO: -6.45454 LUMO: 1.78779 factor:1 | 1 (-2.88511) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.05241 HOMO: -6.84366 LUMO: 1.77690 factor:1 | 1 (-1.75805) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.54371 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-2.24935) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.96590 HOMO: -6.76475 LUMO: 2.40277 factor:1 | 1 (-1.67154) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.91249 HOMO: -6.65863 LUMO: 1.86670 factor:1 | 1 (-1.61813) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.77472 HOMO: -6.50080 LUMO: 1.93201 factor:1 | 1 (-1.48035) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.85270 HOMO: -6.34842 LUMO: 1.70888 factor:1 | 1 (-1.55834) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.94767 HOMO: -6.60692 LUMO: 2.20140 factor:1 | 1 (-1.65331) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.65618 HOMO: -6.74026 LUMO: 2.14970 factor:1 | 1 (-1.36182) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.83484 HOMO: -6.63686 LUMO: 2.17419 factor:1 | 1 (-2.54048) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.10582 HOMO: -6.81917 LUMO: 2.10072 factor:1 | 1 (-1.81146) | 1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.53454 HOMO: -6.92802 LUMO: 2.04358 factor:1 | 1 (-2.24018) | 1 | 1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.47286 HOMO: -6.56067 LUMO: -0.47620 factor:1 | 1 (-1.17850) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.72046 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-1.42609) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.88035 HOMO: -6.78380 LUMO: -0.64763 factor:1 | 1 (-1.58599) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12857.12253 HOMO: -6.51985 LUMO: -0.24490 factor:1 | 1 (-1.82817) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.38374 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-1.08938) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.86416 HOMO: -7.10489 LUMO: -0.62586 factor:1 | 1 (-1.56980) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.87570 HOMO: -7.18108 LUMO: 0.48980 factor:1 | 1 (-1.58134) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.85967 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-1.56531) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.69861 HOMO: -6.70761 LUMO: -0.54423 factor:1 | 1 (-1.40424) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.84693 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-1.55257) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.84334 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-1.54898) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.79493 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-1.50057) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.53098 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-1.23662) | -1 | -1 |
| G: -6590.92867 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12856.82557 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-1.53121) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.30659 HOMO: -6.93890 LUMO: -0.72382 factor:1 | -1 (0.10561) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.54368 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-0.13149) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.27356 HOMO: -6.66951 LUMO: -0.40817 factor:1 | -1 (1.13863) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.59300 HOMO: -6.60420 LUMO: -0.19320 factor:1 | -1 (0.81920) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.42194 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-0.00974) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.97766 HOMO: -7.23823 LUMO: -0.62858 factor:1 | -1 (0.43454) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.66786 HOMO: -7.27088 LUMO: 0.53334 factor:1 | -1 (0.74434) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.40245 HOMO: -7.20013 LUMO: 0.59049 factor:1 | -1 (0.00974) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.84986 HOMO: -6.60148 LUMO: -0.20953 factor:1 | 1 (-0.43767) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.46817 HOMO: -6.69400 LUMO: -0.51974 factor:1 | 1 (-0.05597) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13534.09357 HOMO: -7.40422 LUMO: -0.98777 factor:1 | 1 (-0.68137) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13534.02187 HOMO: -6.88176 LUMO: -0.71022 factor:1 | 1 (-0.60967) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.24199 HOMO: -6.86271 LUMO: -0.59321 factor:1 | -1 (0.17021) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.67509 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-0.26289) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.12808 HOMO: -6.71033 LUMO: 1.57010 factor:1 | -1 (0.28411) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.43843 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-0.02623) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.07000 HOMO: -6.67495 LUMO: 2.03813 factor:1 | -1 (1.34220) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.40488 HOMO: -6.54434 LUMO: 1.83677 factor:1 | -1 (0.00732) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.09306 HOMO: -6.57155 LUMO: 1.77146 factor:1 | -1 (0.31914) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.38548 HOMO: -6.76747 LUMO: 1.87759 factor:1 | -1 (0.02672) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.20740 HOMO: -6.58243 LUMO: 1.61364 factor:1 | -1 (0.20479) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.50335 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-0.09116) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.13383 HOMO: -6.62597 LUMO: 2.00276 factor:1 | -1 (1.27836) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.65242 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-0.24022) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.06585 HOMO: -7.03959 LUMO: 2.16875 factor:1 | -1 (0.34635) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.73833 HOMO: -6.83278 LUMO: 1.91296 factor:1 | -1 (0.67386) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.90538 HOMO: -6.40012 LUMO: 1.95650 factor:1 | -1 (0.50681) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.11794 HOMO: -6.50080 LUMO: 1.73337 factor:1 | -1 (1.29426) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.11225 HOMO: -6.95795 LUMO: 2.28848 factor:1 | -1 (1.29994) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.13462 HOMO: -6.63686 LUMO: 2.20140 factor:1 | -1 (1.27757) | 1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13531.95998 HOMO: -6.57427 LUMO: 1.87214 factor:1 | -1 (1.45222) | 1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13531.98716 HOMO: -6.38379 LUMO: 2.32113 factor:1 | -1 (1.42503) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.18069 HOMO: -6.63958 LUMO: 2.04902 factor:1 | -1 (1.23151) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.80612 HOMO: -6.70216 LUMO: 1.93201 factor:1 | -1 (0.60608) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.75003 HOMO: -6.80557 LUMO: 2.23678 factor:1 | -1 (0.66216) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13534.00750 HOMO: -6.72938 LUMO: 2.28304 factor:1 | 1 (-0.59530) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.86818 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-0.45598) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.27105 HOMO: -6.95523 LUMO: 2.33474 factor:1 | -1 (0.14115) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.22528 HOMO: -6.59876 LUMO: 2.30480 factor:1 | -1 (0.18692) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13534.09444 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-0.68224) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.53136 HOMO: -7.06408 LUMO: 1.99187 factor:1 | 1 (-0.11916) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.78307 HOMO: -6.95795 LUMO: 1.88847 factor:1 | -1 (0.62913) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.66554 HOMO: -6.85455 LUMO: 1.63813 factor:1 | -1 (0.74665) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.87153 HOMO: -7.09129 LUMO: 2.31569 factor:1 | -1 (0.54066) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.69860 HOMO: -6.91441 LUMO: 1.68983 factor:1 | 1 (-0.28640) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.93069 HOMO: -6.89809 LUMO: 2.23678 factor:1 | -1 (0.48151) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.53405 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-0.12185) | 1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.19540 HOMO: -6.94707 LUMO: 2.23678 factor:1 | -1 (0.21679) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.81039 HOMO: -7.07224 LUMO: 2.13337 factor:1 | -1 (0.60181) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.97771 HOMO: -6.94979 LUMO: 2.28031 factor:1 | -1 (0.43448) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13534.01613 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-0.60393) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.19012 HOMO: -6.87360 LUMO: 2.40277 factor:1 | -1 (0.22207) | 1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.30052 HOMO: -6.92802 LUMO: 1.89663 factor:1 | -1 (0.11168) | 1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.72824 HOMO: -6.88448 LUMO: 2.02725 factor:1 | -1 (0.68396) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.62771 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-0.21551) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.22594 HOMO: -6.54978 LUMO: 1.93201 factor:1 | -1 (1.18625) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.49925 HOMO: -6.19331 LUMO: 1.46941 factor:1 | -1 (0.91294) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.38118 HOMO: -6.55794 LUMO: 1.89663 factor:1 | -1 (1.03101) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.17016 HOMO: -6.07630 LUMO: 1.94289 factor:1 | -1 (1.24204) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.76223 HOMO: -7.46408 LUMO: 0.31565 factor:1 | -1 (0.64997) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.90092 HOMO: -6.63958 LUMO: -0.61770 factor:1 | -1 (0.51127) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13531.62128 HOMO: -6.81101 LUMO: -0.57960 factor:1 | -1 (1.79092) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.02774 HOMO: -6.74298 LUMO: -0.57960 factor:1 | -1 (1.38446) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.13348 HOMO: -6.63686 LUMO: -0.42994 factor:1 | -1 (1.27872) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.75461 HOMO: -6.60965 LUMO: -0.41089 factor:1 | -1 (0.65759) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.82802 HOMO: -6.60692 LUMO: -0.80274 factor:1 | -1 (0.58417) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.23645 HOMO: -6.58788 LUMO: -0.78097 factor:1 | -1 (1.17575) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.37721 HOMO: -6.67767 LUMO: -0.48436 factor:1 | -1 (1.03499) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13531.85712 HOMO: -6.63141 LUMO: -0.40545 factor:1 | -1 (1.55508) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.19258 HOMO: -6.62053 LUMO: -0.83811 factor:1 | -1 (1.21961) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.12140 HOMO: -6.59604 LUMO: -0.35375 factor:1 | -1 (1.29080) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.05291 HOMO: -6.34297 LUMO: -0.39729 factor:1 | -1 (1.35929) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.97586 HOMO: -6.67223 LUMO: 1.97827 factor:1 | -1 (0.43633) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.84593 HOMO: -6.40012 LUMO: 1.89935 factor:1 | -1 (0.56627) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.92220 HOMO: -6.74842 LUMO: 1.97283 factor:1 | -1 (0.49000) | 1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.89608 HOMO: -6.76747 LUMO: 2.17147 factor:1 | -1 (0.51612) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.17449 HOMO: -6.72121 LUMO: 1.55649 factor:1 | -1 (1.23771) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.70193 HOMO: -6.97700 LUMO: 2.04085 factor:1 | -1 (0.71027) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.88337 HOMO: -7.06680 LUMO: 2.04085 factor:1 | -1 (0.52883) | 1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13534.07904 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-0.66684) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.96541 HOMO: -6.83006 LUMO: 2.14970 factor:1 | -1 (0.44678) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.32523 HOMO: -6.72665 LUMO: 2.20140 factor:1 | -1 (0.08697) | 1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.81521 HOMO: -6.77291 LUMO: 2.34562 factor:1 | -1 (0.59699) | 1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.01896 HOMO: -6.73754 LUMO: 2.00276 factor:1 | -1 (0.39323) | 1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.85762 HOMO: -7.04231 LUMO: 1.92112 factor:1 | 1 (-0.44542) | 1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.09165 HOMO: -6.83822 LUMO: 1.72248 factor:1 | -1 (0.32055) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.58744 HOMO: -6.57971 LUMO: 2.16603 factor:1 | 1 (-0.17524) | 1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.27696 HOMO: -6.80013 LUMO: 1.88575 factor:1 | -1 (0.13524) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.91899 HOMO: -6.93618 LUMO: 2.18235 factor:1 | -1 (0.49321) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.20808 HOMO: -6.54706 LUMO: 1.91024 factor:1 | -1 (0.20411) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.30286 HOMO: -7.06952 LUMO: 2.18507 factor:1 | -1 (0.10934) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.42616 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-0.01396) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.18588 HOMO: -6.87632 LUMO: 1.92657 factor:1 | -1 (0.22632) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.46836 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-0.05616) | 1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13531.76825 HOMO: -7.17292 LUMO: 1.90752 factor:1 | -1 (1.64395) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13531.93473 HOMO: -6.93890 LUMO: 1.80684 factor:1 | -1 (1.47747) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13534.00916 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-0.59696) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.46025 HOMO: -6.85727 LUMO: 2.13609 factor:1 | 1 (-0.04806) | 1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.85060 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-0.43840) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.71001 HOMO: -6.87360 LUMO: 1.15648 factor:1 | -1 (0.70219) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13531.83429 HOMO: -6.67223 LUMO: 2.07351 factor:1 | -1 (1.57791) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.58624 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-0.17404) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.61563 HOMO: -6.90897 LUMO: 2.28848 factor:1 | 1 (-0.20343) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.61710 HOMO: -7.04231 LUMO: 1.70071 factor:1 | 1 (-0.20490) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.73689 HOMO: -6.69944 LUMO: 1.94834 factor:1 | -1 (0.67530) | 1 | 1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.80383 HOMO: -6.56067 LUMO: 2.20956 factor:1 | -1 (0.60836) | -1 | -1 |
| G: -7269.04650 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.29467 HOMO: -6.65046 LUMO: 2.06807 factor:1 | -1 (0.11753) | 1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.30659 HOMO: -7.08584 LUMO: 1.98915 factor:1 | -1 (0.12700) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.54368 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-0.11010) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.27356 HOMO: -6.62869 LUMO: 2.16331 factor:1 | -1 (1.16002) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.59300 HOMO: -6.85183 LUMO: 2.16058 factor:1 | -1 (0.84059) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.42194 HOMO: -6.54706 LUMO: 1.92384 factor:1 | -1 (0.01165) | -1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.97766 HOMO: -6.84366 LUMO: 2.48984 factor:1 | -1 (0.45593) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.66786 HOMO: -6.77291 LUMO: 2.46263 factor:1 | -1 (0.76573) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.40245 HOMO: -7.01782 LUMO: 2.31025 factor:1 | -1 (0.03113) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.84986 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-0.41628) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.46817 HOMO: -6.64230 LUMO: 1.97283 factor:1 | 1 (-0.03459) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13534.09357 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-0.65998) | -1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13534.02187 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-0.58828) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.24199 HOMO: -7.17020 LUMO: 2.06807 factor:1 | -1 (0.19160) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.67509 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-0.24150) | 1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.12808 HOMO: -7.07496 LUMO: 1.82861 factor:1 | -1 (0.30550) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.43843 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.00484) | 1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.07000 HOMO: -6.92802 LUMO: 1.99187 factor:1 | -1 (1.36359) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.40488 HOMO: -6.69672 LUMO: 2.36739 factor:1 | -1 (0.02871) | 1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.09306 HOMO: -7.13755 LUMO: 2.00276 factor:1 | -1 (0.34052) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.38548 HOMO: -6.92530 LUMO: 2.25582 factor:1 | -1 (0.04811) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.20740 HOMO: -6.77564 LUMO: 1.97827 factor:1 | -1 (0.22618) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.50335 HOMO: -6.87904 LUMO: 1.60003 factor:1 | 1 (-0.06977) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.13383 HOMO: -6.62869 LUMO: 1.90480 factor:1 | -1 (1.29975) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.65242 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-0.21883) | -1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.06585 HOMO: -6.74298 LUMO: 1.47486 factor:1 | -1 (0.36773) | -1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.73833 HOMO: -6.77019 LUMO: 1.90480 factor:1 | -1 (0.69525) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.90538 HOMO: -6.70489 LUMO: 1.99459 factor:1 | -1 (0.52820) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.11794 HOMO: -6.73482 LUMO: 2.08711 factor:1 | -1 (1.31564) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.11225 HOMO: -6.46543 LUMO: 1.73881 factor:1 | -1 (1.32133) | -1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.13462 HOMO: -6.96067 LUMO: 2.26127 factor:1 | -1 (1.29896) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13531.95998 HOMO: -6.67767 LUMO: 2.10616 factor:1 | -1 (1.47361) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13531.98716 HOMO: -6.28855 LUMO: 2.35923 factor:1 | -1 (1.44642) | -1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.18069 HOMO: -6.80285 LUMO: 1.62724 factor:1 | -1 (1.25289) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.80612 HOMO: -6.85455 LUMO: 2.23133 factor:1 | -1 (0.62747) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.75003 HOMO: -6.51713 LUMO: 2.33474 factor:1 | -1 (0.68355) | -1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13534.00750 HOMO: -6.88176 LUMO: 2.15242 factor:1 | 1 (-0.57392) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.86818 HOMO: -6.54434 LUMO: 2.32113 factor:1 | 1 (-0.43459) | -1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.27105 HOMO: -6.62597 LUMO: 2.24222 factor:1 | -1 (0.16253) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.22528 HOMO: -6.74570 LUMO: 2.19868 factor:1 | -1 (0.20830) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13534.09444 HOMO: -6.62869 LUMO: 1.98915 factor:1 | 1 (-0.66086) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.53136 HOMO: -6.64502 LUMO: 2.13881 factor:1 | 1 (-0.09777) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.78307 HOMO: -6.95795 LUMO: 1.82316 factor:1 | -1 (0.65052) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.66554 HOMO: -6.77291 LUMO: 1.36329 factor:1 | -1 (0.76804) | -1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.87153 HOMO: -6.45726 LUMO: 1.73064 factor:1 | -1 (0.56205) | -1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.69860 HOMO: -6.49264 LUMO: 1.77418 factor:1 | 1 (-0.26501) | -1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.93069 HOMO: -6.60420 LUMO: 2.20956 factor:1 | -1 (0.50289) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.53405 HOMO: -6.56067 LUMO: 2.05718 factor:1 | 1 (-0.10046) | -1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.19540 HOMO: -6.62597 LUMO: 1.70343 factor:1 | -1 (0.23818) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.81039 HOMO: -6.69400 LUMO: 2.16875 factor:1 | -1 (0.62320) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.97771 HOMO: -6.63958 LUMO: 2.11977 factor:1 | -1 (0.45587) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13534.01613 HOMO: -6.92802 LUMO: 1.82044 factor:1 | 1 (-0.58254) | 1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.19012 HOMO: -6.56339 LUMO: 2.30480 factor:1 | -1 (0.24346) | -1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.30052 HOMO: -6.63958 LUMO: 1.91024 factor:1 | -1 (0.13306) | 1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.72824 HOMO: -6.93074 LUMO: 2.05446 factor:1 | -1 (0.70535) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.62771 HOMO: -6.61509 LUMO: 2.03813 factor:1 | 1 (-0.19413) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.22594 HOMO: -6.61237 LUMO: 1.91296 factor:1 | -1 (1.20764) | 1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.49925 HOMO: -6.86815 LUMO: 1.95378 factor:1 | -1 (0.93433) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.38118 HOMO: -6.63686 LUMO: 1.70888 factor:1 | -1 (1.05240) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.17016 HOMO: -6.57971 LUMO: 2.20140 factor:1 | -1 (1.26342) | 1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.76223 HOMO: -6.41100 LUMO: 1.96738 factor:1 | -1 (0.67136) | -1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.90092 HOMO: -6.90081 LUMO: 1.65989 factor:1 | -1 (0.53266) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13531.62128 HOMO: -6.68312 LUMO: 1.97827 factor:1 | -1 (1.81231) | 1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.02774 HOMO: -6.65318 LUMO: 2.10888 factor:1 | -1 (1.40585) | 1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.13348 HOMO: -6.62053 LUMO: 2.28848 factor:1 | -1 (1.30011) | 1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.75461 HOMO: -6.65863 LUMO: 2.29664 factor:1 | -1 (0.67898) | 1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.82802 HOMO: -6.63958 LUMO: 2.07623 factor:1 | -1 (0.60556) | 1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.23645 HOMO: -6.58243 LUMO: 2.20684 factor:1 | -1 (1.19714) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.37721 HOMO: -6.59332 LUMO: 2.05174 factor:1 | -1 (1.05637) | 1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13531.85712 HOMO: -6.95251 LUMO: 2.20140 factor:1 | -1 (1.57646) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.19258 HOMO: -6.84638 LUMO: 2.39732 factor:1 | -1 (1.24100) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.12140 HOMO: -6.86815 LUMO: 2.47896 factor:1 | -1 (1.31219) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.05291 HOMO: -7.00693 LUMO: 2.43270 factor:1 | -1 (1.38068) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.97586 HOMO: -6.58788 LUMO: 2.30208 factor:1 | -1 (0.45772) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.84593 HOMO: -6.63958 LUMO: 2.28031 factor:1 | -1 (0.58766) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.92220 HOMO: -6.74570 LUMO: 2.28304 factor:1 | -1 (0.51138) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.89608 HOMO: -6.78380 LUMO: 2.16331 factor:1 | -1 (0.53751) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.17449 HOMO: -6.52529 LUMO: 2.05718 factor:1 | -1 (1.25910) | -1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.70193 HOMO: -6.41644 LUMO: 1.65445 factor:1 | -1 (0.73166) | -1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.88337 HOMO: -6.34570 LUMO: 1.22451 factor:1 | -1 (0.55021) | -1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13534.07904 HOMO: -6.14433 LUMO: 1.85582 factor:1 | 1 (-0.64545) | -1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.96541 HOMO: -6.62053 LUMO: 1.92112 factor:1 | -1 (0.46817) | 1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.32523 HOMO: -6.63414 LUMO: 1.61908 factor:1 | -1 (0.10836) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.81521 HOMO: -6.75931 LUMO: 1.87214 factor:1 | -1 (0.61838) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.01896 HOMO: -6.55794 LUMO: 1.77418 factor:1 | -1 (0.41462) | -1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.85762 HOMO: -6.52801 LUMO: 1.82044 factor:1 | 1 (-0.42404) | -1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.09165 HOMO: -6.77564 LUMO: 1.97827 factor:1 | -1 (0.34194) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.58744 HOMO: -6.93890 LUMO: 1.81228 factor:1 | 1 (-0.15385) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.27696 HOMO: -6.85455 LUMO: 1.75513 factor:1 | -1 (0.15663) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.91899 HOMO: -6.86815 LUMO: 1.64629 factor:1 | -1 (0.51459) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.20808 HOMO: -6.98516 LUMO: 1.84765 factor:1 | -1 (0.22550) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.30286 HOMO: -6.04637 LUMO: 1.94017 factor:1 | -1 (0.13072) | -1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.42616 HOMO: -6.86271 LUMO: 2.11977 factor:1 | -1 (0.00743) | 1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.18588 HOMO: -6.72938 LUMO: 2.11160 factor:1 | -1 (0.24771) | 1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.46836 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-0.03478) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13531.76825 HOMO: -6.18515 LUMO: 2.04630 factor:1 | -1 (1.66534) | -1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13531.93473 HOMO: -6.60965 LUMO: 2.17147 factor:1 | -1 (1.49886) | 1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13534.00916 HOMO: -6.87360 LUMO: 2.35378 factor:1 | 1 (-0.57558) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.46025 HOMO: -6.72938 LUMO: 2.20140 factor:1 | 1 (-0.02667) | 1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.85060 HOMO: -6.88448 LUMO: 2.54154 factor:1 | 1 (-0.41701) | 1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.71001 HOMO: -6.87087 LUMO: 2.16058 factor:1 | -1 (0.72358) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13531.83429 HOMO: -7.11306 LUMO: 2.04085 factor:1 | -1 (1.59929) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.58624 HOMO: -6.66951 LUMO: 1.68438 factor:1 | 1 (-0.15266) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.61563 HOMO: -7.08312 LUMO: 2.19324 factor:1 | 1 (-0.18204) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.61710 HOMO: -6.69128 LUMO: 2.13881 factor:1 | 1 (-0.18351) | 1 | -1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.73689 HOMO: -6.80285 LUMO: 2.16603 factor:1 | -1 (0.69669) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.80383 HOMO: -6.82189 LUMO: 2.46807 factor:1 | -1 (0.62975) | 1 | 1 |
| G: -7269.06789 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.29467 HOMO: -6.78652 LUMO: 2.12521 factor:1 | -1 (0.13891) | 1 | 1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.30659 HOMO: -6.47903 LUMO: 1.70071 factor:1 | 1 (-0.89161) | -1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.54368 HOMO: -6.37019 LUMO: 1.24356 factor:1 | 1 (-1.12870) | -1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.27356 HOMO: -6.69400 LUMO: 1.67350 factor:1 | -1 (0.14142) | 1 | 1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.59300 HOMO: -7.51851 LUMO: 0.27756 factor:1 | 1 (-0.17802) | -1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.42194 HOMO: -6.95795 LUMO: -0.72110 factor:1 | 1 (-1.00696) | -1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.97766 HOMO: -6.88720 LUMO: -0.67484 factor:1 | 1 (-0.56268) | -1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.66786 HOMO: -6.83550 LUMO: -0.57144 factor:1 | 1 (-0.25288) | -1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.40245 HOMO: -6.80285 LUMO: -0.57144 factor:1 | 1 (-0.98747) | -1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.84986 HOMO: -6.76475 LUMO: -0.53062 factor:1 | 1 (-1.43488) | -1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.46817 HOMO: -6.66951 LUMO: 1.74969 factor:1 | 1 (-1.05319) | 1 | 1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13534.09357 HOMO: -6.53345 LUMO: 1.89935 factor:1 | 1 (-1.67859) | -1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13534.02187 HOMO: -6.65046 LUMO: 2.01364 factor:1 | 1 (-1.60689) | 1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.24199 HOMO: -6.64230 LUMO: 2.11977 factor:1 | 1 (-0.82701) | 1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.67509 HOMO: -6.44910 LUMO: 2.13337 factor:1 | 1 (-1.26010) | -1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.12808 HOMO: -7.05591 LUMO: 1.98915 factor:1 | 1 (-0.71310) | 1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.43843 HOMO: -7.02326 LUMO: 2.49256 factor:1 | 1 (-1.02345) | 1 | 1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.07000 HOMO: -6.32937 LUMO: 2.51161 factor:1 | -1 (0.34499) | -1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.40488 HOMO: -6.96067 LUMO: 2.20140 factor:1 | 1 (-0.98990) | 1 | 1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.09306 HOMO: -6.97972 LUMO: 2.55243 factor:1 | 1 (-0.67808) | 1 | 1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.38548 HOMO: -6.72665 LUMO: 2.46535 factor:1 | 1 (-0.97049) | 1 | 1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.20740 HOMO: -6.41917 LUMO: 2.35106 factor:1 | 1 (-0.79242) | -1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.50335 HOMO: -6.75114 LUMO: 2.32929 factor:1 | 1 (-1.08837) | 1 | 1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.13383 HOMO: -6.91713 LUMO: 2.27215 factor:1 | -1 (0.28115) | 1 | 1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.65242 HOMO: -6.54978 LUMO: 2.00276 factor:1 | 1 (-1.23744) | -1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.06585 HOMO: -6.62325 LUMO: 2.05990 factor:1 | 1 (-0.65087) | 1 | 1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.73833 HOMO: -6.86271 LUMO: 2.14970 factor:1 | 1 (-0.32335) | 1 | 1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.90538 HOMO: -6.77564 LUMO: 2.25855 factor:1 | 1 (-0.49040) | 1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.11794 HOMO: -6.71305 LUMO: 1.94561 factor:1 | -1 (0.29704) | 1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.11225 HOMO: -6.75659 LUMO: 1.94561 factor:1 | -1 (0.30273) | 1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.13462 HOMO: -6.94979 LUMO: 2.33474 factor:1 | -1 (0.28036) | 1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13531.95998 HOMO: -6.85727 LUMO: 2.50345 factor:1 | -1 (0.45500) | 1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13531.98716 HOMO: -6.87360 LUMO: 2.43270 factor:1 | -1 (0.42782) | 1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.18069 HOMO: -6.57427 LUMO: 2.46807 factor:1 | -1 (0.23429) | 1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.80612 HOMO: -7.16204 LUMO: 2.15242 factor:1 | 1 (-0.39114) | 1 | 1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.75003 HOMO: -6.62869 LUMO: 2.11432 factor:1 | 1 (-0.33505) | 1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13534.00750 HOMO: -7.05591 LUMO: 2.26671 factor:1 | 1 (-1.59252) | 1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.86818 HOMO: -7.13483 LUMO: 1.47758 factor:1 | 1 (-1.45320) | -1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.27105 HOMO: -6.72938 LUMO: 1.57282 factor:1 | 1 (-0.85607) | -1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.22528 HOMO: -6.17426 LUMO: 1.81228 factor:1 | 1 (-0.81030) | -1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13534.09444 HOMO: -6.65318 LUMO: 1.93473 factor:1 | 1 (-1.67946) | 1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.53136 HOMO: -6.18515 LUMO: 2.01364 factor:1 | 1 (-1.11637) | -1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.78307 HOMO: -7.05591 LUMO: 2.13337 factor:1 | 1 (-0.36809) | 1 | 1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.66554 HOMO: -6.90897 LUMO: 2.29664 factor:1 | 1 (-0.25056) | 1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.87153 HOMO: -7.11034 LUMO: 2.17147 factor:1 | 1 (-0.45655) | 1 | 1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.69860 HOMO: -6.82734 LUMO: 2.26671 factor:1 | 1 (-1.28362) | 1 | 1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.93069 HOMO: -6.34842 LUMO: 2.34562 factor:1 | 1 (-0.51571) | -1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.53405 HOMO: -6.62053 LUMO: 2.22861 factor:1 | 1 (-1.11907) | 1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.19540 HOMO: -6.80557 LUMO: 2.07079 factor:1 | 1 (-0.78042) | 1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.81039 HOMO: -6.60692 LUMO: 2.46263 factor:1 | 1 (-0.39541) | 1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.97771 HOMO: -7.02054 LUMO: 2.08711 factor:1 | 1 (-0.56273) | 1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13534.01613 HOMO: -6.78652 LUMO: 2.02453 factor:1 | 1 (-1.60115) | 1 | 1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.19012 HOMO: -6.51168 LUMO: 2.06534 factor:1 | 1 (-0.77514) | -1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.30052 HOMO: -6.50080 LUMO: 2.01636 factor:1 | 1 (-0.88554) | -1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.72824 HOMO: -6.54434 LUMO: 1.84493 factor:1 | 1 (-0.31326) | -1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.62771 HOMO: -6.47087 LUMO: 1.76330 factor:1 | 1 (-1.21273) | -1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.22594 HOMO: -6.78924 LUMO: 2.39460 factor:1 | -1 (0.18904) | 1 | 1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.49925 HOMO: -6.59876 LUMO: 1.84493 factor:1 | 1 (-0.08427) | 1 | 1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.38118 HOMO: -6.41644 LUMO: 2.05174 factor:1 | -1 (0.03380) | -1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.17016 HOMO: -6.52257 LUMO: 2.11160 factor:1 | -1 (0.24482) | -1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.76223 HOMO: -6.90897 LUMO: 2.34018 factor:1 | 1 (-0.34724) | 1 | 1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.90092 HOMO: -6.97428 LUMO: 1.86126 factor:1 | 1 (-0.48594) | 1 | 1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13531.62128 HOMO: -7.13483 LUMO: 2.14698 factor:1 | -1 (0.79370) | 1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.02774 HOMO: -7.16748 LUMO: 2.31841 factor:1 | -1 (0.38725) | 1 | 1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.13348 HOMO: -6.87087 LUMO: 2.38916 factor:1 | -1 (0.28150) | 1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.75461 HOMO: -6.93074 LUMO: 2.42181 factor:1 | 1 (-0.33963) | 1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.82802 HOMO: -6.90081 LUMO: 2.00276 factor:1 | 1 (-0.41304) | 1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.23645 HOMO: -6.99333 LUMO: 2.03541 factor:1 | -1 (0.17853) | 1 | 1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.37721 HOMO: -6.89264 LUMO: 1.57554 factor:1 | -1 (0.03777) | -1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13531.85712 HOMO: -6.48175 LUMO: 1.85854 factor:1 | -1 (0.55786) | -1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.19258 HOMO: -6.69400 LUMO: 1.62452 factor:1 | -1 (0.22240) | 1 | 1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.12140 HOMO: -6.50896 LUMO: 1.88303 factor:1 | -1 (0.29358) | -1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.05291 HOMO: -6.60420 LUMO: 2.05990 factor:1 | -1 (0.36207) | 1 | 1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.97586 HOMO: -7.14299 LUMO: 2.07351 factor:1 | 1 (-0.56088) | 1 | 1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.84593 HOMO: -7.06408 LUMO: 1.81228 factor:1 | 1 (-0.43095) | 1 | 1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.92220 HOMO: -6.67495 LUMO: 1.79595 factor:1 | 1 (-0.50722) | 1 | 1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.89608 HOMO: -6.45182 LUMO: 2.15786 factor:1 | 1 (-0.48110) | -1 | -1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.17449 HOMO: -6.93346 LUMO: 2.45719 factor:1 | -1 (0.24049) | 1 | 1 |
| G: -7268.04929 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.70193 HOMO: -6.50080 LUMO: 2.08167 factor:1 | 1 (-0.28694) | -1 | -1 |
| G: -7268.04929 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.88337 HOMO: -6.83550 LUMO: -0.67484 factor:1 | 1 (-0.46839) | -1 | -1 |
| G: -7268.04929 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13534.07904 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-1.66406) | -1 | -1 |
| G: -7268.04929 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.96541 HOMO: -6.79740 LUMO: 1.91296 factor:1 | 1 (-0.55043) | -1 | -1 |
| G: -7268.04929 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.32523 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-0.91025) | -1 | -1 |
| G: -7268.04929 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.81521 HOMO: -6.62597 LUMO: -0.44082 factor:1 | 1 (-0.40023) | -1 | -1 |
| G: -7268.04929 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.01896 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-0.60398) | -1 | -1 |
| G: -7268.04929 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.85762 HOMO: -6.51168 LUMO: -0.23130 factor:1 | 1 (-1.44264) | -1 | -1 |
| G: -7268.04929 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.09165 HOMO: -7.14027 LUMO: 0.49797 factor:1 | 1 (-0.67667) | -1 | -1 |
| G: -7268.04929 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.58744 HOMO: -7.55660 LUMO: 0.24762 factor:1 | 1 (-1.17246) | -1 | -1 |
| G: -7268.04929 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.27696 HOMO: -6.88992 LUMO: -0.64763 factor:1 | 1 (-0.86198) | -1 | -1 |
| G: -7268.04929 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.91899 HOMO: -6.72665 LUMO: -0.45987 factor:1 | 1 (-0.50401) | -1 | -1 |
| G: -7268.04929 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.20808 HOMO: -6.72121 LUMO: -0.58232 factor:1 | 1 (-0.79310) | -1 | -1 |
| G: -7268.04929 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.30286 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-0.88788) | -1 | -1 |
| G: -7268.04929 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.42616 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-1.01118) | -1 | -1 |
| G: -7268.04929 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.18588 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-0.77090) | -1 | -1 |
| G: -7268.04929 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.46836 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-1.05338) | -1 | -1 |
| G: -7268.04929 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13531.76825 HOMO: -6.77019 LUMO: -0.62858 factor:1 | -1 (0.64673) | -1 | -1 |
| G: -7268.04929 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13531.93473 HOMO: -6.82462 LUMO: -0.67484 factor:1 | -1 (0.48025) | -1 | -1 |
| G: -7268.04929 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13534.00916 HOMO: -6.79740 LUMO: -0.55511 factor:1 | 1 (-1.59418) | -1 | -1 |
| G: -7268.04929 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.46025 HOMO: -6.79740 LUMO: -0.67756 factor:1 | 1 (-1.04527) | -1 | -1 |
| G: -7268.04929 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.85060 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-1.43562) | -1 | -1 |
| G: -7268.04929 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.71001 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-0.29503) | -1 | -1 |
| G: -7268.04929 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13531.83429 HOMO: -6.48992 LUMO: -0.25034 factor:1 | -1 (0.58069) | -1 | -1 |
| G: -7268.04929 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.58624 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-1.17126) | -1 | -1 |
| G: -7268.04929 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.61563 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-1.20065) | -1 | -1 |
| G: -7268.04929 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.61710 HOMO: -6.59332 LUMO: -0.27211 factor:1 | 1 (-1.20212) | -1 | -1 |
| G: -7268.04929 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.73689 HOMO: -6.57427 LUMO: -0.16871 factor:1 | 1 (-0.32191) | -1 | -1 |
| G: -7268.04929 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.80383 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-0.38885) | -1 | -1 |
| G: -7268.04929 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.29467 HOMO: -6.72121 LUMO: 2.00004 factor:1 | 1 (-0.87969) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.30659 HOMO: -6.61509 LUMO: 1.55921 factor:1 | 1 (-1.10310) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.54368 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-1.34019) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.27356 HOMO: -6.66135 LUMO: 2.02181 factor:1 | 1 (-0.07007) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.59300 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-0.38950) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.42194 HOMO: -6.66679 LUMO: 1.98371 factor:1 | 1 (-1.21844) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.97766 HOMO: -6.67495 LUMO: 2.04085 factor:1 | 1 (-0.77416) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.66786 HOMO: -6.89809 LUMO: 1.95106 factor:1 | 1 (-0.46436) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.40245 HOMO: -6.50352 LUMO: 1.88847 factor:1 | 1 (-1.19896) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.84986 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-1.64637) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.46817 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-1.26468) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13534.09357 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-1.89008) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13534.02187 HOMO: -6.65591 LUMO: 2.20684 factor:1 | 1 (-1.81837) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.24199 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-1.03850) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.67509 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-1.47159) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.12808 HOMO: -6.53617 LUMO: 1.75241 factor:1 | 1 (-0.92459) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.43843 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-1.23493) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.07000 HOMO: -7.40422 LUMO: -0.97145 factor:1 | -1 (0.13350) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.40488 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-1.20138) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.09306 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-0.88957) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.38548 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-1.18198) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.20740 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-1.00391) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.50335 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-1.29986) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.13383 HOMO: -7.29265 LUMO: 0.48164 factor:1 | -1 (0.06966) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.65242 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-1.44892) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.06585 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-0.86236) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.73833 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-0.53484) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.90538 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-0.70189) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.11794 HOMO: -6.90897 LUMO: 1.91296 factor:1 | -1 (0.08555) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.11225 HOMO: -6.67495 LUMO: 2.04358 factor:1 | -1 (0.09124) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.13462 HOMO: -6.94162 LUMO: 1.73881 factor:1 | -1 (0.06887) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13531.95998 HOMO: -6.73482 LUMO: 1.95922 factor:1 | -1 (0.24351) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13531.98716 HOMO: -6.70489 LUMO: 2.04358 factor:1 | -1 (0.21633) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.18069 HOMO: -7.04231 LUMO: 1.79323 factor:1 | -1 (0.02280) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.80612 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-0.60262) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.75003 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-0.54654) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13534.00750 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-1.80401) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.86818 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-1.66468) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.27105 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-1.06756) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.22528 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-1.02179) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13534.09444 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-1.89095) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.53136 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-1.32786) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.78307 HOMO: -6.75387 LUMO: 1.72248 factor:1 | 1 (-0.57958) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.66554 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-0.46205) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.87153 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-0.66804) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.69860 HOMO: -6.80557 LUMO: 2.02725 factor:1 | 1 (-1.49510) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.93069 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-0.72720) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.53405 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-1.33056) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.19540 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-0.99191) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.81039 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-0.60690) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.97771 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-0.77422) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13534.01613 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-1.81263) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.19012 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-0.98663) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.30052 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-1.09703) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.72824 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-0.52474) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.62771 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-1.42422) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.22594 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-0.02245) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.49925 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-0.29576) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.38118 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-0.17769) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.17016 HOMO: -6.58788 LUMO: 1.79051 factor:1 | -1 (0.03333) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.76223 HOMO: -6.64230 LUMO: 2.16058 factor:1 | 1 (-0.55873) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.90092 HOMO: -6.58788 LUMO: 2.10616 factor:1 | 1 (-0.69743) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13531.62128 HOMO: -7.01782 LUMO: 2.13609 factor:1 | -1 (0.58221) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.02774 HOMO: -6.31304 LUMO: 2.31841 factor:1 | -1 (0.17576) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.13348 HOMO: -6.94979 LUMO: 2.07895 factor:1 | -1 (0.07001) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.75461 HOMO: -6.88992 LUMO: 2.28031 factor:1 | 1 (-0.55111) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.82802 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-0.62453) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.23645 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-0.03295) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.37721 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-0.17372) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13531.85712 HOMO: -6.55250 LUMO: 1.95378 factor:1 | -1 (0.34637) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.19258 HOMO: -6.24773 LUMO: 1.77962 factor:1 | -1 (0.01091) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.12140 HOMO: -6.31304 LUMO: 2.18507 factor:1 | -1 (0.08210) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.05291 HOMO: -6.18243 LUMO: 2.01636 factor:1 | -1 (0.15059) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.97586 HOMO: -6.99877 LUMO: 2.14970 factor:1 | 1 (-0.77237) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.84593 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-0.64243) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.92220 HOMO: -6.36202 LUMO: 2.17419 factor:1 | 1 (-0.71871) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.89608 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-0.69258) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.17449 HOMO: -6.87360 LUMO: 2.34290 factor:1 | -1 (0.02901) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.70193 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-0.49843) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.88337 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-0.67988) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13534.07904 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-1.87554) | 1 | 1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.96541 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-0.76192) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.32523 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-1.12173) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.81521 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-0.61171) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.01896 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-0.81547) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.85762 HOMO: -6.44094 LUMO: 1.74425 factor:1 | 1 (-1.65413) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.09165 HOMO: -6.51985 LUMO: 1.84221 factor:1 | 1 (-0.88815) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.58744 HOMO: -6.63414 LUMO: -0.24762 factor:1 | 1 (-1.38394) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.27696 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-1.07346) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.91899 HOMO: -7.19741 LUMO: 0.58232 factor:1 | 1 (-0.71550) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.20808 HOMO: -6.77019 LUMO: -0.56872 factor:1 | 1 (-1.00459) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.30286 HOMO: -7.46136 LUMO: 0.28844 factor:1 | 1 (-1.09937) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.42616 HOMO: -6.60420 LUMO: -0.54151 factor:1 | 1 (-1.22266) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.18588 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-0.98239) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.46836 HOMO: -6.81645 LUMO: -0.57144 factor:1 | 1 (-1.26487) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13531.76825 HOMO: -7.48041 LUMO: 0.28572 factor:1 | -1 (0.43525) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13531.93473 HOMO: -6.75659 LUMO: -0.45715 factor:1 | -1 (0.26877) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13534.00916 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-1.80567) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.46025 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-1.25676) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.85060 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-1.64711) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.71001 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-0.50651) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13531.83429 HOMO: -6.53617 LUMO: -0.25579 factor:1 | -1 (0.36920) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.58624 HOMO: -6.50896 LUMO: -0.25034 factor:1 | 1 (-1.38275) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.61563 HOMO: -7.17564 LUMO: -0.68573 factor:1 | 1 (-1.41213) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.61710 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-1.41360) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.73689 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-0.53340) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13532.80383 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-0.60034) | -1 | -1 |
| G: -7267.83780 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13533.29467 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-1.09118) | -1 | -1 |
| G: -7164.94393 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13429.93519 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-0.62556) | -1 | -1 |
| G: -7164.94393 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13429.85459 HOMO: -6.62325 LUMO: 2.02725 factor:1 | 1 (-0.54496) | -1 | -1 |
| G: -7164.94393 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13430.00926 HOMO: -6.63414 LUMO: 1.91296 factor:1 | 1 (-0.69963) | -1 | -1 |
| G: -7164.94393 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13430.13492 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-0.82529) | -1 | -1 |
| G: -7164.94393 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13430.15756 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-0.84793) | -1 | -1 |
| G: -7165.00211 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13429.93519 HOMO: -6.61237 LUMO: 2.11432 factor:1 | 1 (-0.56738) | -1 | -1 |
| G: -7165.00211 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13429.85459 HOMO: -6.62053 LUMO: 2.09256 factor:1 | 1 (-0.48678) | -1 | -1 |
| G: -7165.00211 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13430.00926 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-0.64145) | -1 | -1 |
| G: -7165.00211 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13430.13492 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-0.76712) | -1 | -1 |
| G: -7165.00211 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13430.15756 HOMO: -6.85183 LUMO: 2.12793 factor:1 | 1 (-0.78976) | -1 | -1 |
| G: -7706.19100 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13970.93319 HOMO: -6.81101 LUMO: 1.83949 factor:1 | 1 (-0.37650) | -1 | -1 |
| G: -7706.19100 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13970.79988 HOMO: -6.98788 LUMO: 2.16058 factor:1 | 1 (-0.24319) | -1 | -1 |
| G: -7706.19100 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13970.99673 HOMO: -6.62869 LUMO: 2.00820 factor:1 | 1 (-0.44004) | -1 | -1 |
| G: -7706.19100 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13970.94225 HOMO: -6.34025 LUMO: 2.25855 factor:1 | 1 (-0.38556) | -1 | -1 |
| G: -7706.19100 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13970.87014 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-0.31345) | -1 | -1 |
| G: -7706.19100 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13970.75792 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-0.20123) | -1 | -1 |
| G: -7706.19100 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13970.99150 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-0.43481) | -1 | -1 |
| G: -7706.19100 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13971.23137 HOMO: -6.83278 LUMO: 1.53744 factor:1 | 1 (-0.67468) | -1 | -1 |
| G: -7706.19100 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13971.12840 HOMO: -6.41917 LUMO: 1.82316 factor:1 | 1 (-0.57171) | -1 | -1 |
| G: -7705.84669 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13970.93319 HOMO: -6.56339 LUMO: 1.63813 factor:1 | 1 (-0.72080) | -1 | -1 |
| G: -7705.84669 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13970.79988 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-0.58749) | -1 | -1 |
| G: -7705.84669 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13970.99673 HOMO: -6.63141 LUMO: 1.92112 factor:1 | 1 (-0.78434) | -1 | -1 |
| G: -7705.84669 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13970.94225 HOMO: -6.83822 LUMO: 1.88847 factor:1 | 1 (-0.72986) | -1 | -1 |
| G: -7705.84669 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13970.87014 HOMO: -6.84638 LUMO: 1.90480 factor:1 | 1 (-0.65775) | -1 | -1 |
| G: -7705.84669 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13970.75792 HOMO: -6.82462 LUMO: 1.70888 factor:1 | 1 (-0.54553) | -1 | -1 |
| G: -7705.84669 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13970.99150 HOMO: -6.82734 LUMO: 2.12521 factor:1 | 1 (-0.77912) | -1 | -1 |
| G: -7705.84669 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13971.23137 HOMO: -6.94435 LUMO: 1.87214 factor:1 | 1 (-1.01898) | -1 | -1 |
| G: -7705.84669 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13971.12840 HOMO: -6.98516 LUMO: 2.51433 factor:1 | 1 (-0.91602) | -1 | -1 |
| G: -7706.47843 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13970.93319 HOMO: -6.74026 LUMO: 2.15514 factor:1 | 1 (-0.08906) | -1 | -1 |
| G: -7706.47843 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13970.79988 HOMO: -6.93618 LUMO: 2.54426 factor:1 | -1 (0.04425) | -1 | -1 |
| G: -7706.47843 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13970.99673 HOMO: -6.28583 LUMO: 2.53610 factor:1 | 1 (-0.15260) | -1 | -1 |
| G: -7706.47843 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13970.94225 HOMO: -6.56883 LUMO: 1.94834 factor:1 | 1 (-0.09812) | -1 | -1 |
| G: -7706.47843 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13970.87014 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-0.02601) | 1 | 1 |
| G: -7706.47843 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13970.75792 HOMO: -6.19059 LUMO: 1.99732 factor:1 | -1 (0.08621) | -1 | -1 |
| G: -7706.47843 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13970.99150 HOMO: -6.78108 LUMO: 2.03813 factor:1 | 1 (-0.14738) | -1 | -1 |
| G: -7706.47843 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13971.23137 HOMO: -6.82189 LUMO: 1.77418 factor:1 | 1 (-0.38725) | -1 | -1 |
| G: -7706.47843 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -13971.12840 HOMO: -6.45454 LUMO: 1.78779 factor:1 | 1 (-0.28428) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03352 HOMO: -6.84366 LUMO: 1.77690 factor:1 | 1 (-0.57919) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84902 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-0.39470) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.57944 HOMO: -6.76475 LUMO: 2.40277 factor:1 | 1 (-0.12512) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.44220 HOMO: -6.65863 LUMO: 1.86670 factor:1 | 1 (-1.98787) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.06807 HOMO: -6.50080 LUMO: 1.93201 factor:1 | 1 (-1.61374) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.01581 HOMO: -6.34842 LUMO: 1.70888 factor:1 | 1 (-2.56149) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14426 HOMO: -6.60692 LUMO: 2.20140 factor:1 | 1 (-1.68994) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.29803 HOMO: -6.74026 LUMO: 2.14970 factor:1 | 1 (-1.84371) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87095 HOMO: -6.63686 LUMO: 2.17419 factor:1 | 1 (-1.41662) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91870 HOMO: -6.81917 LUMO: 2.10072 factor:1 | 1 (-1.46438) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90734 HOMO: -6.92802 LUMO: 2.04358 factor:1 | 1 (-0.45302) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31279 HOMO: -6.56067 LUMO: -0.47620 factor:1 | 1 (-0.85846) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94470 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-0.49038) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26729 HOMO: -6.78380 LUMO: -0.64763 factor:1 | 1 (-0.81297) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20982 HOMO: -6.51985 LUMO: -0.24490 factor:1 | 1 (-0.75550) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.44933 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-0.99501) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.61638 HOMO: -7.10489 LUMO: -0.62586 factor:1 | 1 (-1.16206) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80545 HOMO: -7.18108 LUMO: 0.48980 factor:1 | 1 (-1.35113) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94529 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-1.49097) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.65973 HOMO: -6.70761 LUMO: -0.54423 factor:1 | 1 (-1.20541) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.23591 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-0.78159) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.16650 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-0.71218) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.81999 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-0.36567) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.19684 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-0.74252) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.95011 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-0.49579) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.75980 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-0.30548) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04078 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-0.58646) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.98805 HOMO: -6.66951 LUMO: -0.40817 factor:1 | 1 (-0.53372) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.40693 HOMO: -6.60420 LUMO: -0.19320 factor:1 | 1 (-1.95261) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71807 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-1.26375) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81658 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-1.36226) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02926 HOMO: -7.27088 LUMO: 0.53334 factor:1 | 1 (-1.57494) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.34372 HOMO: -7.20013 LUMO: 0.59049 factor:1 | 1 (-1.88940) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.21977 HOMO: -6.60148 LUMO: -0.20953 factor:1 | 1 (-1.76545) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.26497 HOMO: -6.69400 LUMO: -0.51974 factor:1 | 1 (-1.81065) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.14668 HOMO: -7.40422 LUMO: -0.98777 factor:1 | 1 (-1.69236) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03763 HOMO: -6.88176 LUMO: -0.71022 factor:1 | 1 (-0.58330) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.87120 HOMO: -6.86271 LUMO: -0.59321 factor:1 | 1 (-0.41688) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07972 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-0.62540) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.43659 HOMO: -6.71033 LUMO: 1.57010 factor:1 | 1 (-1.98227) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90921 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-1.45488) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80221 HOMO: -6.67495 LUMO: 2.03813 factor:1 | 1 (-1.34789) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90619 HOMO: -6.54434 LUMO: 1.83677 factor:1 | 1 (-1.45186) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00703 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-1.55271) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87946 HOMO: -6.76747 LUMO: 1.87759 factor:1 | 1 (-1.42514) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13657 HOMO: -6.58243 LUMO: 1.61364 factor:1 | 1 (-0.68224) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05120 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-0.59688) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.94410 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-0.48978) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12138 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-0.66706) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.04282 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-0.58850) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.03874 HOMO: -6.83278 LUMO: 1.91296 factor:1 | 1 (-0.58442) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05523 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-0.60091) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92949 HOMO: -6.50080 LUMO: 1.73337 factor:1 | 1 (-0.47517) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12590 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-0.67158) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08603 HOMO: -6.63686 LUMO: 2.20140 factor:1 | 1 (-0.63171) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.07700 HOMO: -6.57427 LUMO: 1.87214 factor:1 | 1 (-0.62268) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.84032 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-0.38599) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02666 HOMO: -6.63958 LUMO: 2.04902 factor:1 | 1 (-0.57234) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.85101 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-0.39669) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06329 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-0.60896) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.05184 HOMO: -6.72938 LUMO: 2.28304 factor:1 | 1 (-2.59752) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.24889 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-1.79456) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.30391 HOMO: -6.95523 LUMO: 2.33474 factor:1 | 1 (-1.84959) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.91966 HOMO: -6.59876 LUMO: 2.30480 factor:1 | 1 (-0.46534) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90990 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-0.45557) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92821 HOMO: -7.06408 LUMO: 1.99187 factor:1 | 1 (-0.47389) | 1 | 1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01300 HOMO: -6.95795 LUMO: 1.88847 factor:1 | 1 (-0.55868) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.36530 HOMO: -6.85455 LUMO: 1.63813 factor:1 | 1 (-1.91097) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.72863 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-1.27431) | 1 | 1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.93634 HOMO: -6.91441 LUMO: 1.68983 factor:1 | 1 (-1.48201) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.90281 HOMO: -6.89809 LUMO: 2.23678 factor:1 | 1 (-1.44849) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89751 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-1.44318) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.93692 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-0.48259) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06900 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-0.61468) | 1 | 1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92396 HOMO: -6.94979 LUMO: 2.28031 factor:1 | 1 (-0.46964) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15140 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-0.69707) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18797 HOMO: -6.87360 LUMO: 2.40277 factor:1 | 1 (-0.73365) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.46615 HOMO: -6.92802 LUMO: 1.89663 factor:1 | 1 (-1.01183) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13589 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-0.68156) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.33159 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-0.87727) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22342 HOMO: -6.54978 LUMO: 1.93201 factor:1 | 1 (-0.76910) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13433 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-0.68001) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.29834 HOMO: -6.55794 LUMO: 1.89663 factor:1 | 1 (-0.84402) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22571 HOMO: -6.07630 LUMO: 1.94289 factor:1 | 1 (-0.77139) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12233 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-0.66801) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17338 HOMO: -6.63958 LUMO: -0.61770 factor:1 | 1 (-0.71906) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99752 HOMO: -6.81101 LUMO: -0.57960 factor:1 | 1 (-0.54319) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.02682 HOMO: -6.74298 LUMO: -0.57960 factor:1 | 1 (-0.57250) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08987 HOMO: -6.63686 LUMO: -0.42994 factor:1 | 1 (-0.63555) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17028 HOMO: -6.60965 LUMO: -0.41089 factor:1 | 1 (-0.71596) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.28193 HOMO: -6.60692 LUMO: -0.80274 factor:1 | 1 (-0.82761) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.68126 HOMO: -6.58788 LUMO: -0.78097 factor:1 | 1 (-1.22693) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.87073 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-1.41641) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.64139 HOMO: -6.63141 LUMO: -0.40545 factor:1 | 1 (-1.18707) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89272 HOMO: -6.62053 LUMO: -0.83811 factor:1 | 1 (-1.43839) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.62999 HOMO: -6.59604 LUMO: -0.35375 factor:1 | 1 (-1.17567) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.95459 HOMO: -6.34297 LUMO: -0.39729 factor:1 | 1 (-1.50027) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05490 HOMO: -6.67223 LUMO: 1.97827 factor:1 | 1 (-0.60058) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99806 HOMO: -6.40012 LUMO: 1.89935 factor:1 | 1 (-0.54374) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06497 HOMO: -6.74842 LUMO: 1.97283 factor:1 | 1 (-0.61065) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12217 HOMO: -6.76747 LUMO: 2.17147 factor:1 | 1 (-0.66785) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.08105 HOMO: -6.72121 LUMO: 1.55649 factor:1 | 1 (-0.62673) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15738 HOMO: -6.97700 LUMO: 2.04085 factor:1 | 1 (-0.70306) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.20478 HOMO: -7.06680 LUMO: 2.04085 factor:1 | 1 (-0.75046) | 1 | 1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15923 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-0.70491) | 1 | 1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.50906 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-1.05474) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31507 HOMO: -6.72665 LUMO: 2.20140 factor:1 | 1 (-0.86075) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22440 HOMO: -6.77291 LUMO: 2.34562 factor:1 | 1 (-0.77008) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.26255 HOMO: -6.73754 LUMO: 2.00276 factor:1 | 1 (-0.80823) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.25654 HOMO: -7.04231 LUMO: 1.92112 factor:1 | 1 (-0.80222) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.12729 HOMO: -6.83822 LUMO: 1.72248 factor:1 | 1 (-0.67296) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22789 HOMO: -6.57971 LUMO: 2.16603 factor:1 | 1 (-0.77357) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.18367 HOMO: -6.80013 LUMO: 1.88575 factor:1 | 1 (-0.72935) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.06089 HOMO: -6.93618 LUMO: 2.18235 factor:1 | 1 (-0.60657) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70915 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-1.25483) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.97250 HOMO: -7.06952 LUMO: 2.18507 factor:1 | 1 (-1.51818) | 1 | 1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.98733 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-1.53301) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.89506 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-1.44073) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.00728 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-1.55295) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.81571 HOMO: -7.17292 LUMO: 1.90752 factor:1 | 1 (-1.36139) | 1 | 1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.80836 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-1.35404) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.17161 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-0.71729) | 1 | 1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.31047 HOMO: -6.85727 LUMO: 2.13609 factor:1 | 1 (-0.85615) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.22168 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-0.76736) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.13526 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-0.68094) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58749 HOMO: -6.67223 LUMO: 2.07351 factor:1 | 1 (-1.13316) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71002 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-1.25570) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.74716 HOMO: -6.90897 LUMO: 2.28848 factor:1 | 1 (-1.29284) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88082 HOMO: -7.04231 LUMO: 1.70071 factor:1 | 1 (-1.42650) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.70433 HOMO: -6.69944 LUMO: 1.94834 factor:1 | 1 (-1.25001) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.57698 HOMO: -6.56067 LUMO: 2.20956 factor:1 | 1 (-1.12266) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.69598 HOMO: -6.65046 LUMO: 2.06807 factor:1 | 1 (-1.24166) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.75065 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-1.29632) | 1 | 1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.51976 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-1.06543) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.58476 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-1.13044) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.88763 HOMO: -6.85183 LUMO: 2.16058 factor:1 | 1 (-1.43331) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91780 HOMO: -6.54706 LUMO: 1.92384 factor:1 | 1 (-1.46348) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.67233 HOMO: -6.84366 LUMO: 2.48984 factor:1 | 1 (-1.21801) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.71426 HOMO: -6.77291 LUMO: 2.46263 factor:1 | 1 (-1.25994) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.38712 HOMO: -7.01782 LUMO: 2.31025 factor:1 | 1 (-1.93280) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11579.11660 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-2.66228) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.42862 HOMO: -6.64230 LUMO: 1.97283 factor:1 | 1 (-1.97429) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91500 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-1.46068) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91029 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-1.45597) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.02831 HOMO: -7.17020 LUMO: 2.06807 factor:1 | 1 (-1.57399) | 1 | 1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.37950 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-1.92518) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.22298 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-1.76866) | 1 | 1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.33262 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-1.87829) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.01199 HOMO: -6.92802 LUMO: 1.99187 factor:1 | 1 (-0.55767) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90432 HOMO: -6.69672 LUMO: 2.36739 factor:1 | 1 (-0.44999) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.92502 HOMO: -7.13755 LUMO: 2.00276 factor:1 | 1 (-0.47070) | 1 | 1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.15861 HOMO: -6.92530 LUMO: 2.25582 factor:1 | 1 (-0.70429) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11578.59148 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-2.13716) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.94219 HOMO: -6.87904 LUMO: 1.60003 factor:1 | 1 (-1.48786) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.91201 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-1.45769) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.96205 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-1.50773) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.99577 HOMO: -6.74298 LUMO: 1.47486 factor:1 | 1 (-0.54145) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11576.90045 HOMO: -6.77019 LUMO: 1.90480 factor:1 | 1 (-0.44613) | -1 | -1 |
| G: -5312.08863 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11577.05071 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-0.59639) | -1 | -1 |