乙二醇作为反应物的反应表19-13

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: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87488 HOMO: -6.91169 LUMO: -0.53879 factor:1 | 1 (-0.20904) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.71496 HOMO: -7.29809 LUMO: 2.83543 factor:1 | 1 (-0.04912) | 1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25609 HOMO: -6.86543 LUMO: -0.70205 factor:1 | 1 (-0.59024) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.26847 HOMO: -7.47769 LUMO: 0.31293 factor:1 | 1 (-0.60262) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25726 HOMO: -6.63141 LUMO: -0.55511 factor:1 | 1 (-0.59141) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.55950 HOMO: -6.68856 LUMO: -0.30205 factor:1 | 1 (-0.89365) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.27750 HOMO: -7.22190 LUMO: 0.53334 factor:1 | 1 (-0.61166) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.05668 HOMO: -6.66407 LUMO: -0.27756 factor:1 | 1 (-0.39084) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.28020 HOMO: -7.15659 LUMO: -0.70205 factor:1 | 1 (-0.61435) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25345 HOMO: -6.69400 LUMO: 1.67622 factor:1 | 1 (-0.58760) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.24047 HOMO: -6.60420 LUMO: 2.16058 factor:1 | 1 (-0.57462) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.15372 HOMO: -6.87087 LUMO: 1.88031 factor:1 | 1 (-0.48787) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.50673 HOMO: -6.60965 LUMO: -0.19864 factor:1 | 1 (-0.84089) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.96751 HOMO: -7.29265 LUMO: 0.52246 factor:1 | 1 (-0.30167) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.84860 HOMO: -6.86543 LUMO: -0.59593 factor:1 | 1 (-0.18275) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.30618 HOMO: -7.44504 LUMO: -1.01226 factor:1 | 1 (-0.64034) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.20618 HOMO: -6.92530 LUMO: -0.75103 factor:1 | 1 (-0.54034) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.13051 HOMO: -7.10489 LUMO: 2.20412 factor:1 | 1 (-0.46466) | 1 | 1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.23707 HOMO: -6.58788 LUMO: 1.73881 factor:1 | 1 (-0.57122) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.26311 HOMO: -6.64502 LUMO: 1.70343 factor:1 | 1 (-0.59726) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.41620 HOMO: -6.73754 LUMO: 1.60819 factor:1 | 1 (-0.75035) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.26063 HOMO: -6.80829 LUMO: 2.45991 factor:1 | 1 (-0.59479) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.15424 HOMO: -6.91713 LUMO: 2.43814 factor:1 | 1 (-0.48839) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.99440 HOMO: -6.60692 LUMO: 1.93745 factor:1 | 1 (-0.32855) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92346 HOMO: -6.26134 LUMO: 1.46125 factor:1 | 1 (-0.25761) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.88335 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-0.21750) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.78201 HOMO: -6.97700 LUMO: -0.73471 factor:1 | 1 (-0.11617) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.15486 HOMO: -6.92258 LUMO: -0.70205 factor:1 | 1 (-0.48902) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.10692 HOMO: -6.83550 LUMO: -0.56872 factor:1 | 1 (-0.44107) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92781 HOMO: -6.72121 LUMO: 1.89663 factor:1 | 1 (-0.26196) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.13135 HOMO: -6.73482 LUMO: 1.89935 factor:1 | 1 (-0.46551) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09598 HOMO: -6.61781 LUMO: 1.86670 factor:1 | 1 (-0.43013) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.12313 HOMO: -7.01782 LUMO: 2.26399 factor:1 | 1 (-0.45729) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25592 HOMO: -7.23551 LUMO: 2.09800 factor:1 | 1 (-0.59008) | 1 | 1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02115 HOMO: -7.13483 LUMO: 2.17963 factor:1 | 1 (-0.35530) | 1 | 1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14732 HOMO: -6.22869 LUMO: 2.01092 factor:1 | 1 (-0.48148) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.03222 HOMO: -6.80285 LUMO: 2.14970 factor:1 | 1 (-0.36637) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.46102 HOMO: -7.21102 LUMO: 2.33746 factor:1 | 1 (-0.79517) | 1 | 1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.22452 HOMO: -6.39740 LUMO: 2.59597 factor:1 | 1 (-0.55868) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.97997 HOMO: -7.07768 LUMO: 2.48168 factor:1 | 1 (-0.31413) | 1 | 1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09211 HOMO: -7.11306 LUMO: 0.90614 factor:1 | 1 (-0.42627) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92218 HOMO: -6.61781 LUMO: -2.46263 factor:1 | 1 (-0.25633) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.24069 HOMO: -6.96611 LUMO: 0.90614 factor:1 | 1 (-0.57484) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17103 HOMO: -6.86271 LUMO: -1.14832 factor:1 | 1 (-0.50518) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09023 HOMO: -6.72665 LUMO: 0.96873 factor:1 | 1 (-0.42439) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.96008 HOMO: -7.14571 LUMO: 1.05036 factor:1 | 1 (-0.29424) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.82209 HOMO: -7.14299 LUMO: 0.98777 factor:1 | 1 (-0.15625) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.70702 HOMO: -6.99333 LUMO: 1.05852 factor:1 | 1 (-0.04117) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87921 HOMO: -6.78924 LUMO: -1.49935 factor:1 | 1 (-0.21336) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.93298 HOMO: -7.13755 LUMO: 0.94151 factor:1 | 1 (-0.26713) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87023 HOMO: -6.72938 LUMO: -0.35375 factor:1 | 1 (-0.20438) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.72898 HOMO: -6.99061 LUMO: 0.82450 factor:1 | 1 (-0.06313) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.15573 HOMO: -6.75114 LUMO: -0.68028 factor:1 | 1 (-0.48989) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09238 HOMO: -6.40556 LUMO: -0.42722 factor:1 | 1 (-0.42654) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.06384 HOMO: -7.18653 LUMO: 0.42178 factor:1 | 1 (-0.39799) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.86680 HOMO: -6.63958 LUMO: -0.71294 factor:1 | 1 (-0.20096) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.32458 HOMO: -6.63958 LUMO: -0.71022 factor:1 | 1 (-0.65873) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14493 HOMO: -6.69672 LUMO: -0.72654 factor:1 | 1 (-0.47908) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16504 HOMO: -6.56883 LUMO: -0.80274 factor:1 | 1 (-0.49919) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16931 HOMO: -6.68584 LUMO: -0.56872 factor:1 | 1 (-0.50347) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.43917 HOMO: -6.59060 LUMO: -0.35647 factor:1 | 1 (-0.77332) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.32082 HOMO: -6.72121 LUMO: -0.71838 factor:1 | 1 (-0.65498) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04438 HOMO: -6.57971 LUMO: -0.61498 factor:1 | 1 (-0.37854) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.90727 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-0.24142) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92781 HOMO: -7.14027 LUMO: 0.43266 factor:1 | 1 (-0.26196) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.15992 HOMO: -6.43277 LUMO: -0.44082 factor:1 | 1 (-0.49408) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.91513 HOMO: -6.79468 LUMO: 0.07619 factor:1 | 1 (-0.24928) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14077 HOMO: -6.81917 LUMO: -2.57148 factor:1 | 1 (-0.47492) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01617 HOMO: -6.71849 LUMO: 1.30615 factor:1 | 1 (-0.35032) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.23979 HOMO: -6.85455 LUMO: -0.63675 factor:1 | 1 (-0.57394) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.21674 HOMO: -6.73210 LUMO: -1.03131 factor:1 | 1 (-0.55089) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17590 HOMO: -6.83550 LUMO: -0.58777 factor:1 | 1 (-0.51005) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.38063 HOMO: -6.53073 LUMO: -0.74287 factor:1 | 1 (-0.71479) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.05679 HOMO: -7.18381 LUMO: -0.92791 factor:1 | 1 (-0.39095) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.99641 HOMO: -6.49264 LUMO: -0.44627 factor:1 | 1 (-0.33056) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.32379 HOMO: -7.32803 LUMO: 0.41361 factor:1 | 1 (-0.65794) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.86724 HOMO: -6.53073 LUMO: -0.52790 factor:1 | 1 (-0.20139) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.79698 HOMO: -6.54978 LUMO: -0.53062 factor:1 | 1 (-0.13113) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.71689 HOMO: -6.56611 LUMO: -0.37824 factor:1 | 1 (-0.05105) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.23720 HOMO: -6.57155 LUMO: -0.64219 factor:1 | 1 (-0.57136) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.20458 HOMO: -7.08040 LUMO: 0.45715 factor:1 | 1 (-0.53873) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.18972 HOMO: -6.66679 LUMO: -0.75376 factor:1 | 1 (-0.52387) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.39903 HOMO: -6.83550 LUMO: -0.99322 factor:1 | 1 (-0.73318) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04860 HOMO: -6.53345 LUMO: -0.29660 factor:1 | 1 (-0.38276) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04817 HOMO: -6.65046 LUMO: 2.40549 factor:1 | 1 (-0.38232) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.97418 HOMO: -6.98788 LUMO: 2.01092 factor:1 | 1 (-0.30833) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01423 HOMO: -6.61781 LUMO: 1.92384 factor:1 | 1 (-0.34839) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.88128 HOMO: -6.61237 LUMO: 2.06807 factor:1 | 1 (-0.21543) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.08267 HOMO: -6.59060 LUMO: 1.95106 factor:1 | 1 (-0.41682) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.95831 HOMO: -6.48175 LUMO: 1.72248 factor:1 | 1 (-0.29247) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14996 HOMO: -6.84911 LUMO: 2.03541 factor:1 | 1 (-0.48412) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.12879 HOMO: -6.50624 LUMO: 2.17147 factor:1 | 1 (-0.46295) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.20569 HOMO: -6.68312 LUMO: 2.08439 factor:1 | 1 (-0.53985) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16332 HOMO: -6.96067 LUMO: 1.98099 factor:1 | 1 (-0.49748) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87333 HOMO: -6.93618 LUMO: 1.85854 factor:1 | 1 (-0.20749) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.82492 HOMO: -6.71305 LUMO: -0.61226 factor:1 | 1 (-0.15908) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.70122 HOMO: -7.06408 LUMO: 0.80001 factor:1 | 1 (-0.03537) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.95222 HOMO: -6.52257 LUMO: 0.99049 factor:1 | 1 (-0.28637) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.81992 HOMO: -6.84638 LUMO: 1.10750 factor:1 | 1 (-0.15407) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.63292 HOMO: -6.85455 LUMO: 0.84900 factor:1 | -1 (0.03293) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.90495 HOMO: -6.60148 LUMO: -0.78369 factor:1 | 1 (-0.23911) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01562 HOMO: -6.86543 LUMO: -0.93063 factor:1 | 1 (-0.34978) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.96452 HOMO: -6.70489 LUMO: -0.72382 factor:1 | 1 (-0.29867) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.18221 HOMO: -6.59060 LUMO: 0.31293 factor:1 | 1 (-0.51636) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.75333 HOMO: -6.52257 LUMO: -0.48708 factor:1 | 1 (-0.08748) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.00743 HOMO: -6.54706 LUMO: -0.48164 factor:1 | 1 (-0.34158) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.90416 HOMO: -7.32803 LUMO: 0.08436 factor:1 | 1 (-0.23832) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.03804 HOMO: -6.77291 LUMO: -0.66940 factor:1 | 1 (-0.37220) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16414 HOMO: -6.68312 LUMO: -0.53062 factor:1 | 1 (-0.49829) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.24741 HOMO: -7.07768 LUMO: 0.45987 factor:1 | 1 (-0.58156) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.05489 HOMO: -6.50352 LUMO: -0.63675 factor:1 | 1 (-0.38904) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.37337 HOMO: -6.48992 LUMO: -0.60681 factor:1 | 1 (-0.70752) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.13470 HOMO: -6.65318 LUMO: -0.72382 factor:1 | 1 (-0.46885) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.05238 HOMO: -6.54706 LUMO: 0.24218 factor:1 | 1 (-0.38654) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.93488 HOMO: -6.63958 LUMO: 0.57416 factor:1 | 1 (-0.26904) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.31906 HOMO: -6.37563 LUMO: -0.48164 factor:1 | 1 (-0.65321) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92688 HOMO: -6.64774 LUMO: -0.71838 factor:1 | 1 (-0.26104) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.84351 HOMO: -7.17020 LUMO: 0.45987 factor:1 | 1 (-0.17766) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.73877 HOMO: -6.86543 LUMO: -1.05036 factor:1 | 1 (-0.07293) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.13905 HOMO: -6.77019 LUMO: -1.03131 factor:1 | 1 (-0.47321) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19685 HOMO: -6.80285 LUMO: 1.05852 factor:1 | 1 (-0.53100) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16787 HOMO: -6.76475 LUMO: 1.01771 factor:1 | 1 (-0.50202) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.46178 HOMO: -6.92530 LUMO: 1.37417 factor:1 | 1 (-0.79593) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25873 HOMO: -6.98244 LUMO: 1.25989 factor:1 | 1 (-0.59288) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17415 HOMO: -6.74842 LUMO: 0.89798 factor:1 | 1 (-0.50831) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14071 HOMO: -6.77019 LUMO: -1.17009 factor:1 | 1 (-0.47487) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.95148 HOMO: -6.78652 LUMO: 1.35785 factor:1 | 1 (-0.28564) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01083 HOMO: -6.82734 LUMO: -0.68301 factor:1 | 1 (-0.34499) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.00787 HOMO: -6.48175 LUMO: -2.19052 factor:1 | 1 (-0.34202) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19168 HOMO: -6.65863 LUMO: -0.77008 factor:1 | 1 (-0.52583) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.23791 HOMO: -6.44094 LUMO: -2.20956 factor:1 | 1 (-0.57206) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04798 HOMO: -6.59876 LUMO: -0.57688 factor:1 | 1 (-0.38213) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17467 HOMO: -6.78380 LUMO: -0.77008 factor:1 | 1 (-0.50883) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.24763 HOMO: -7.30354 LUMO: 0.25034 factor:1 | 1 (-0.58178) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02925 HOMO: -6.59332 LUMO: -0.53334 factor:1 | 1 (-0.36341) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.13630 HOMO: -6.64230 LUMO: -0.55783 factor:1 | 1 (-0.47046) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.90547 HOMO: -7.26544 LUMO: 0.20409 factor:1 | 1 (-0.23962) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.12403 HOMO: -6.61237 LUMO: -0.65307 factor:1 | 1 (-0.45819) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92683 HOMO: -6.72393 LUMO: -0.65307 factor:1 | 1 (-0.26098) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01540 HOMO: -6.29671 LUMO: -0.39729 factor:1 | 1 (-0.34956) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.85159 HOMO: -6.75387 LUMO: -0.53334 factor:1 | 1 (-0.18574) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04866 HOMO: -6.53073 LUMO: -0.31293 factor:1 | 1 (-0.38281) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.86686 HOMO: -6.42189 LUMO: -0.59049 factor:1 | 1 (-0.20101) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.81072 HOMO: -6.41100 LUMO: -0.29933 factor:1 | 1 (-0.14487) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.66941 HOMO: -6.57427 LUMO: -0.53879 factor:1 | 1 (-0.00356) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.12479 HOMO: -7.43143 LUMO: 0.33470 factor:1 | 1 (-0.45895) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92645 HOMO: -6.56067 LUMO: -0.50885 factor:1 | 1 (-0.26060) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.71687 HOMO: -6.65863 LUMO: -0.76464 factor:1 | 1 (-0.05102) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02000 HOMO: -6.32665 LUMO: -0.41906 factor:1 | 1 (-0.35416) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.82326 HOMO: -6.57699 LUMO: 1.63813 factor:1 | 1 (-0.15742) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.18474 HOMO: -6.53073 LUMO: 1.71704 factor:1 | 1 (-0.51889) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02425 HOMO: -6.86271 LUMO: 2.07351 factor:1 | 1 (-0.35840) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.18354 HOMO: -6.63686 LUMO: 1.78235 factor:1 | 1 (-0.51770) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.11456 HOMO: -6.60965 LUMO: 1.94289 factor:1 | 1 (-0.44872) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.73349 HOMO: -6.55250 LUMO: 1.89119 factor:1 | 1 (-0.06765) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14166 HOMO: -6.50624 LUMO: 1.85582 factor:1 | 1 (-0.47582) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09179 HOMO: -6.06814 LUMO: 1.94561 factor:1 | 1 (-0.42594) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.30305 HOMO: -6.58788 LUMO: 2.01908 factor:1 | 1 (-0.63721) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.37024 HOMO: -6.74026 LUMO: 0.31293 factor:1 | 1 (-0.70439) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25579 HOMO: -6.54434 LUMO: -0.42994 factor:1 | 1 (-0.58994) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.10471 HOMO: -6.94707 LUMO: 0.42994 factor:1 | 1 (-0.43887) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.88337 HOMO: -6.98516 LUMO: 0.41361 factor:1 | 1 (-0.21753) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.08047 HOMO: -6.31304 LUMO: -0.54967 factor:1 | 1 (-0.41462) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.08572 HOMO: -6.48447 LUMO: -0.40817 factor:1 | 1 (-0.41987) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09391 HOMO: -6.49264 LUMO: 0.29116 factor:1 | 1 (-0.42806) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.88343 HOMO: -6.48719 LUMO: -0.11973 factor:1 | 1 (-0.21758) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.24303 HOMO: -7.16204 LUMO: 0.44082 factor:1 | 1 (-0.57718) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.03940 HOMO: -6.74842 LUMO: -0.37552 factor:1 | 1 (-0.37356) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.32017 HOMO: -6.44638 LUMO: -0.45171 factor:1 | 1 (-0.65432) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17837 HOMO: -7.07496 LUMO: 0.50341 factor:1 | 1 (-0.51253) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04196 HOMO: -6.79468 LUMO: 0.11429 factor:1 | 1 (-0.37612) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.90405 HOMO: -6.63958 LUMO: -0.67484 factor:1 | 1 (-0.23821) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17426 HOMO: -7.08584 LUMO: 0.46259 factor:1 | 1 (-0.50842) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02716 HOMO: -6.80285 LUMO: -0.73199 factor:1 | 1 (-0.36131) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.93080 HOMO: -6.44366 LUMO: -0.45443 factor:1 | 1 (-0.26496) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19622 HOMO: -6.75931 LUMO: 0.25851 factor:1 | 1 (-0.53038) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.97954 HOMO: -6.64502 LUMO: 1.79323 factor:1 | 1 (-0.31369) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87916 HOMO: -6.51168 LUMO: 1.60275 factor:1 | 1 (-0.21331) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.78416 HOMO: -6.56067 LUMO: 1.63268 factor:1 | 1 (-0.11832) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.08776 HOMO: -6.56883 LUMO: 1.70615 factor:1 | 1 (-0.42191) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04112 HOMO: -6.77836 LUMO: 1.77962 factor:1 | 1 (-0.37527) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.12063 HOMO: -6.38923 LUMO: 1.85854 factor:1 | 1 (-0.45478) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.24077 HOMO: -6.35658 LUMO: 2.16875 factor:1 | 1 (-0.57492) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16909 HOMO: -6.83006 LUMO: 2.31025 factor:1 | 1 (-0.50325) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.18188 HOMO: -6.87087 LUMO: 1.79051 factor:1 | 1 (-0.51604) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.18934 HOMO: -6.56339 LUMO: 2.37828 factor:1 | 1 (-0.52349) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.03078 HOMO: -6.30488 LUMO: 2.51705 factor:1 | 1 (-0.36493) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04847 HOMO: -6.69400 LUMO: 1.95650 factor:1 | 1 (-0.38262) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.89839 HOMO: -6.51168 LUMO: 2.03541 factor:1 | 1 (-0.23255) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.82857 HOMO: -6.30760 LUMO: 1.65173 factor:1 | 1 (-0.16272) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09902 HOMO: -6.55250 LUMO: 1.90752 factor:1 | 1 (-0.43318) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.99665 HOMO: -6.41372 LUMO: 1.76058 factor:1 | 1 (-0.33081) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.78813 HOMO: -6.23957 LUMO: 2.06534 factor:1 | 1 (-0.12229) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02357 HOMO: -6.58243 LUMO: 2.11705 factor:1 | 1 (-0.35772) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.80661 HOMO: -6.37835 LUMO: 2.09256 factor:1 | 1 (-0.14076) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.93714 HOMO: -6.50624 LUMO: 2.55787 factor:1 | 1 (-0.27130) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02183 HOMO: -6.45454 LUMO: 1.87214 factor:1 | 1 (-0.35598) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.83499 HOMO: -6.53617 LUMO: 1.95650 factor:1 | 1 (-0.16915) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.96229 HOMO: -6.51985 LUMO: 1.71432 factor:1 | 1 (-0.29644) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87624 HOMO: -6.75114 LUMO: 1.84493 factor:1 | 1 (-0.21040) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.68196 HOMO: -6.06270 LUMO: 1.65717 factor:1 | 1 (-0.01611) | -1 | -1 |
| G: -5345.30015 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.06613 HOMO: -5.89671 LUMO: 1.71704 factor:1 | 1 (-0.40028) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.46015 HOMO: -6.18787 LUMO: 1.91840 factor:1 | 1 (-0.82170) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.39288 HOMO: -6.01644 LUMO: 1.85582 factor:1 | 1 (-0.75444) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19614 HOMO: -6.05998 LUMO: 2.33474 factor:1 | 1 (-0.55770) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.32518 HOMO: -6.05725 LUMO: 2.03541 factor:1 | 1 (-0.68673) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.40232 HOMO: -6.80829 LUMO: 1.90480 factor:1 | 1 (-0.76388) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.22809 HOMO: -6.76475 LUMO: 2.20956 factor:1 | 1 (-0.58964) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.44472 HOMO: -6.29944 LUMO: 1.77962 factor:1 | 1 (-0.80627) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.33541 HOMO: -6.47359 LUMO: -0.25579 factor:1 | 1 (-0.69697) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.33829 HOMO: -6.57699 LUMO: -0.47348 factor:1 | 1 (-0.69985) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.46793 HOMO: -7.20830 LUMO: 0.49797 factor:1 | 1 (-0.82948) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.37819 HOMO: -7.49402 LUMO: 0.29933 factor:1 | 1 (-0.73974) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.48050 HOMO: -6.66679 LUMO: -0.58777 factor:1 | 1 (-0.84206) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.27761 HOMO: -6.67767 LUMO: -0.56328 factor:1 | 1 (-0.63917) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.20224 HOMO: -7.42871 LUMO: 0.35647 factor:1 | 1 (-0.56379) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.41351 HOMO: -6.56067 LUMO: -0.54423 factor:1 | 1 (-0.77506) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.28352 HOMO: -6.56339 LUMO: -0.50341 factor:1 | 1 (-0.64507) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.03230 HOMO: -6.56067 LUMO: -0.48436 factor:1 | 1 (-0.39386) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.15867 HOMO: -6.73210 LUMO: 1.75241 factor:1 | 1 (-0.52023) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.03559 HOMO: -6.48175 LUMO: 1.91296 factor:1 | 1 (-0.39715) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19018 HOMO: -6.67767 LUMO: 1.70343 factor:1 | 1 (-0.55174) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.08047 HOMO: -6.37835 LUMO: 1.96466 factor:1 | 1 (-0.44202) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.34978 HOMO: -6.40828 LUMO: 2.10072 factor:1 | 1 (-0.71133) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16871 HOMO: -6.06542 LUMO: 1.92112 factor:1 | 1 (-0.53027) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.32183 HOMO: -6.90353 LUMO: 1.83133 factor:1 | 1 (-0.68339) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19024 HOMO: -6.37019 LUMO: 1.92929 factor:1 | 1 (-0.55179) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14953 HOMO: -6.61509 LUMO: 2.11160 factor:1 | 1 (-0.51108) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.49574 HOMO: -6.82734 LUMO: 1.77146 factor:1 | 1 (-0.85729) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19609 HOMO: -6.01100 LUMO: 1.89935 factor:1 | 1 (-0.55764) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.86596 HOMO: -6.49536 LUMO: 1.75241 factor:1 | 1 (-0.22751) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.05053 HOMO: -6.34297 LUMO: 1.86398 factor:1 | 1 (-0.41209) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.08131 HOMO: -6.53073 LUMO: 1.84493 factor:1 | 1 (-0.44287) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.29005 HOMO: -6.53345 LUMO: 2.41093 factor:1 | 1 (-0.65160) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14599 HOMO: -7.01237 LUMO: 2.06262 factor:1 | 1 (-0.50755) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92182 HOMO: -6.17154 LUMO: 1.89119 factor:1 | 1 (-0.28338) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.89121 HOMO: -6.08719 LUMO: 1.74425 factor:1 | 1 (-0.25277) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.11658 HOMO: -6.69672 LUMO: 1.95106 factor:1 | 1 (-0.47813) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17854 HOMO: -6.58243 LUMO: 2.24766 factor:1 | 1 (-0.54009) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09864 HOMO: -6.74570 LUMO: 2.02181 factor:1 | 1 (-0.46020) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25282 HOMO: -6.53890 LUMO: 1.92929 factor:1 | 1 (-0.61438) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17445 HOMO: -6.03276 LUMO: 1.67078 factor:1 | 1 (-0.53601) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.06705 HOMO: -6.67767 LUMO: 2.03541 factor:1 | 1 (-0.42861) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.38050 HOMO: -5.98378 LUMO: 1.84221 factor:1 | 1 (-0.74205) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.81532 HOMO: -6.07086 LUMO: 2.01908 factor:1 | 1 (-0.17687) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.86971 HOMO: -6.29944 LUMO: 1.90208 factor:1 | 1 (-0.23127) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.82174 HOMO: -6.75114 LUMO: 1.85854 factor:1 | 1 (-0.18330) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17728 HOMO: -6.56611 LUMO: 2.49801 factor:1 | 1 (-0.53884) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16615 HOMO: -6.39740 LUMO: 1.92929 factor:1 | 1 (-0.52771) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.11524 HOMO: -6.85999 LUMO: -1.07757 factor:1 | 1 (-0.47680) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.37451 HOMO: -6.98244 LUMO: 1.07213 factor:1 | 1 (-0.73607) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.28776 HOMO: -7.04231 LUMO: 0.64219 factor:1 | 1 (-0.64932) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.34627 HOMO: -6.96339 LUMO: 0.75648 factor:1 | 1 (-0.70782) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01929 HOMO: -6.83822 LUMO: -0.97417 factor:1 | 1 (-0.38085) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14224 HOMO: -6.44910 LUMO: -2.15242 factor:1 | 1 (-0.50379) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01021 HOMO: -6.84094 LUMO: -1.37690 factor:1 | 1 (-0.37176) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87540 HOMO: -6.74026 LUMO: -2.54699 factor:1 | 1 (-0.23696) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16009 HOMO: -6.96611 LUMO: 1.24900 factor:1 | 1 (-0.52164) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.95641 HOMO: -7.21102 LUMO: 0.82995 factor:1 | 1 (-0.31797) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.97616 HOMO: -6.88448 LUMO: 0.81634 factor:1 | 1 (-0.33772) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.11252 HOMO: -7.04231 LUMO: 1.10750 factor:1 | 1 (-0.47408) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.11723 HOMO: -6.83550 LUMO: -0.98777 factor:1 | 1 (-0.47878) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87488 HOMO: -6.82189 LUMO: 0.93879 factor:1 | 1 (-0.23644) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.71496 HOMO: -6.81101 LUMO: 0.70750 factor:1 | 1 (-0.07652) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25609 HOMO: -7.06680 LUMO: 0.74015 factor:1 | 1 (-0.61764) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.26847 HOMO: -6.68856 LUMO: 0.86260 factor:1 | 1 (-0.63003) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25726 HOMO: -6.83822 LUMO: -0.63403 factor:1 | 1 (-0.61881) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.55950 HOMO: -6.84911 LUMO: 1.26533 factor:1 | 1 (-0.92105) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.27750 HOMO: -7.01237 LUMO: 0.73743 factor:1 | 1 (-0.63906) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.05668 HOMO: -7.00965 LUMO: 1.40139 factor:1 | 1 (-0.41824) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.28020 HOMO: -6.73210 LUMO: -2.49256 factor:1 | 1 (-0.64175) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25345 HOMO: -7.08040 LUMO: 0.84627 factor:1 | 1 (-0.61500) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.24047 HOMO: -7.00965 LUMO: 0.82995 factor:1 | 1 (-0.60202) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.15372 HOMO: -6.88448 LUMO: 0.82723 factor:1 | 1 (-0.51527) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.50673 HOMO: -7.20013 LUMO: 0.88437 factor:1 | 1 (-0.86829) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.96751 HOMO: -6.60420 LUMO: -0.53334 factor:1 | 1 (-0.32907) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.84860 HOMO: -6.78652 LUMO: -0.79729 factor:1 | 1 (-0.21015) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.30618 HOMO: -6.48992 LUMO: -0.64491 factor:1 | 1 (-0.66774) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.20618 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-0.56774) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.13051 HOMO: -6.65046 LUMO: -0.78097 factor:1 | 1 (-0.49206) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.23707 HOMO: -7.24095 LUMO: 0.37280 factor:1 | 1 (-0.59862) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.26311 HOMO: -6.81101 LUMO: -0.74831 factor:1 | 1 (-0.62466) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.41620 HOMO: -6.69400 LUMO: -0.77280 factor:1 | 1 (-0.77776) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.26063 HOMO: -6.08447 LUMO: -0.68573 factor:1 | 1 (-0.62219) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.15424 HOMO: -6.66679 LUMO: -0.47076 factor:1 | 1 (-0.51579) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.99440 HOMO: -6.97428 LUMO: -1.10750 factor:1 | 1 (-0.35595) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92346 HOMO: -6.69128 LUMO: -0.54151 factor:1 | 1 (-0.28501) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.88335 HOMO: -6.53617 LUMO: -0.35375 factor:1 | 1 (-0.24490) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.78201 HOMO: -6.75659 LUMO: -0.41361 factor:1 | 1 (-0.14357) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.15486 HOMO: -6.69400 LUMO: -0.67484 factor:1 | 1 (-0.51642) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.10692 HOMO: -6.89264 LUMO: -0.90886 factor:1 | 1 (-0.46847) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92781 HOMO: -6.56339 LUMO: -0.52518 factor:1 | 1 (-0.28937) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.13135 HOMO: -6.45726 LUMO: -0.65852 factor:1 | 1 (-0.49291) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09598 HOMO: -6.80557 LUMO: -0.56600 factor:1 | 1 (-0.45753) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.12313 HOMO: -7.19469 LUMO: -0.91702 factor:1 | 1 (-0.48469) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25592 HOMO: -6.41100 LUMO: 0.79185 factor:1 | 1 (-0.61748) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02115 HOMO: -6.39195 LUMO: 0.26123 factor:1 | 1 (-0.38270) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14732 HOMO: -6.78924 LUMO: 0.35919 factor:1 | 1 (-0.50888) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.03222 HOMO: -6.50624 LUMO: 0.71838 factor:1 | 1 (-0.39378) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.46102 HOMO: -6.68584 LUMO: -0.66124 factor:1 | 1 (-0.82257) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.22452 HOMO: -6.45182 LUMO: -0.48980 factor:1 | 1 (-0.58608) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.97997 HOMO: -7.18925 LUMO: -1.01498 factor:1 | 1 (-0.34153) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09211 HOMO: -7.18925 LUMO: -0.63130 factor:1 | 1 (-0.45367) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92218 HOMO: -6.66679 LUMO: -0.57960 factor:1 | 1 (-0.28373) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.24069 HOMO: -6.44910 LUMO: -0.30205 factor:1 | 1 (-0.60224) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17103 HOMO: -7.23279 LUMO: 0.46804 factor:1 | 1 (-0.53258) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09023 HOMO: -6.92802 LUMO: -0.72927 factor:1 | 1 (-0.45179) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.96008 HOMO: -6.83278 LUMO: -0.59321 factor:1 | 1 (-0.32164) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.82209 HOMO: -7.44776 LUMO: 0.27211 factor:1 | 1 (-0.18365) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.70702 HOMO: -6.80829 LUMO: -0.59865 factor:1 | 1 (-0.06857) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87921 HOMO: -6.63686 LUMO: -0.75103 factor:1 | 1 (-0.24077) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.93298 HOMO: -6.73210 LUMO: -0.55511 factor:1 | 1 (-0.29454) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87023 HOMO: -6.50624 LUMO: 1.58642 factor:1 | 1 (-0.23179) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.72898 HOMO: -6.79196 LUMO: 0.96328 factor:1 | 1 (-0.09053) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.15573 HOMO: -6.82734 LUMO: 1.23540 factor:1 | 1 (-0.51729) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09238 HOMO: -6.90081 LUMO: 1.25444 factor:1 | 1 (-0.45394) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.06384 HOMO: -7.00965 LUMO: -1.05036 factor:1 | 1 (-0.42540) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.86680 HOMO: -7.01237 LUMO: -1.48302 factor:1 | 1 (-0.22836) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.32458 HOMO: -6.91713 LUMO: 0.93607 factor:1 | 1 (-0.68614) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14493 HOMO: -7.02598 LUMO: 0.92247 factor:1 | 1 (-0.50649) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16504 HOMO: -6.98516 LUMO: 1.52384 factor:1 | 1 (-0.52659) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16931 HOMO: -6.75387 LUMO: 1.04764 factor:1 | 1 (-0.53087) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.43917 HOMO: -7.09401 LUMO: 1.19458 factor:1 | 1 (-0.80072) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.32082 HOMO: -6.88992 LUMO: -1.56193 factor:1 | 1 (-0.68238) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04438 HOMO: -7.00149 LUMO: 0.99866 factor:1 | 1 (-0.40594) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.90727 HOMO: -7.13755 LUMO: 1.05308 factor:1 | 1 (-0.26882) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92781 HOMO: -6.85183 LUMO: -1.42860 factor:1 | 1 (-0.28937) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.15992 HOMO: -6.63141 LUMO: -0.88981 factor:1 | 1 (-0.52148) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.91513 HOMO: -6.92258 LUMO: -0.82178 factor:1 | 1 (-0.27669) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14077 HOMO: -6.55794 LUMO: -0.80818 factor:1 | 1 (-0.50232) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01617 HOMO: -6.95251 LUMO: -0.97145 factor:1 | 1 (-0.37772) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.23979 HOMO: -7.37701 LUMO: 0.14150 factor:1 | 1 (-0.60134) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.21674 HOMO: -6.74842 LUMO: -0.68028 factor:1 | 1 (-0.57830) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17590 HOMO: -6.65046 LUMO: -0.52518 factor:1 | 1 (-0.53745) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.38063 HOMO: -6.91441 LUMO: -1.13199 factor:1 | 1 (-0.74219) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.05679 HOMO: -7.00965 LUMO: -1.00682 factor:1 | 1 (-0.41835) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.99641 HOMO: -6.55794 LUMO: -0.54967 factor:1 | 1 (-0.35797) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.32379 HOMO: -6.71577 LUMO: -0.53879 factor:1 | 1 (-0.68535) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.86724 HOMO: -6.88992 LUMO: -0.55511 factor:1 | 1 (-0.22879) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.79698 HOMO: -6.74026 LUMO: -0.60681 factor:1 | 1 (-0.15853) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.71689 HOMO: -6.76747 LUMO: -0.50885 factor:1 | 1 (-0.07845) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.23720 HOMO: -6.87904 LUMO: -0.92519 factor:1 | 1 (-0.59876) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.20458 HOMO: -6.53073 LUMO: -0.53062 factor:1 | 1 (-0.56613) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.18972 HOMO: -6.97700 LUMO: -0.98505 factor:1 | 1 (-0.55128) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.39903 HOMO: -6.96884 LUMO: -0.79185 factor:1 | 1 (-0.76059) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04860 HOMO: -6.60420 LUMO: -0.31021 factor:1 | 1 (-0.41016) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04817 HOMO: -6.68584 LUMO: -0.63947 factor:1 | 1 (-0.40972) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.97418 HOMO: -6.41917 LUMO: -0.35103 factor:1 | 1 (-0.33573) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01423 HOMO: -6.73482 LUMO: -0.70477 factor:1 | 1 (-0.37579) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.88128 HOMO: -6.71305 LUMO: -0.85716 factor:1 | 1 (-0.24283) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.08267 HOMO: -6.70761 LUMO: -0.63403 factor:1 | 1 (-0.44423) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.95831 HOMO: -6.37563 LUMO: -0.38640 factor:1 | 1 (-0.31987) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14996 HOMO: -6.27495 LUMO: -0.54967 factor:1 | 1 (-0.51152) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.12879 HOMO: -6.98516 LUMO: 0.38096 factor:1 | 1 (-0.49035) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.20569 HOMO: -6.47087 LUMO: -0.40001 factor:1 | 1 (-0.56725) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16332 HOMO: -6.59876 LUMO: 0.20681 factor:1 | 1 (-0.52488) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87333 HOMO: -6.89809 LUMO: 0.14966 factor:1 | 1 (-0.23489) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.82492 HOMO: -6.76203 LUMO: 2.11432 factor:1 | 1 (-0.18648) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.70122 HOMO: -6.58516 LUMO: 1.75786 factor:1 | 1 (-0.06278) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.95222 HOMO: -6.37835 LUMO: 1.84493 factor:1 | 1 (-0.31377) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.81992 HOMO: -6.83550 LUMO: 1.74425 factor:1 | 1 (-0.18147) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.63292 HOMO: -6.65318 LUMO: 1.79051 factor:1 | -1 (0.00552) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.90495 HOMO: -6.68584 LUMO: 2.11160 factor:1 | 1 (-0.26651) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01562 HOMO: -6.36202 LUMO: 1.85037 factor:1 | 1 (-0.37718) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.96452 HOMO: -6.68312 LUMO: 2.23133 factor:1 | 1 (-0.32607) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.18221 HOMO: -6.66679 LUMO: 2.14154 factor:1 | 1 (-0.54377) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.75333 HOMO: -6.50896 LUMO: 1.92657 factor:1 | 1 (-0.11489) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.00743 HOMO: -6.63686 LUMO: 2.22317 factor:1 | 1 (-0.36899) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.90416 HOMO: -6.58788 LUMO: 2.17419 factor:1 | 1 (-0.26572) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.03804 HOMO: -6.72665 LUMO: 2.12249 factor:1 | 1 (-0.39960) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16414 HOMO: -6.28311 LUMO: 1.91024 factor:1 | 1 (-0.52570) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.24741 HOMO: -6.56067 LUMO: 2.27487 factor:1 | 1 (-0.60896) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.05489 HOMO: -6.83006 LUMO: 2.28031 factor:1 | 1 (-0.41644) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.37337 HOMO: -6.45182 LUMO: 1.62724 factor:1 | 1 (-0.73493) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.13470 HOMO: -6.78380 LUMO: 1.83677 factor:1 | 1 (-0.49625) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.05238 HOMO: -6.23413 LUMO: 1.80956 factor:1 | 1 (-0.41394) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.93488 HOMO: -6.74298 LUMO: 2.16875 factor:1 | 1 (-0.29644) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.31906 HOMO: -6.81645 LUMO: 2.50073 factor:1 | 1 (-0.68061) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92688 HOMO: -6.71033 LUMO: 1.96466 factor:1 | 1 (-0.28844) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.84351 HOMO: -6.83550 LUMO: 2.04358 factor:1 | 1 (-0.20507) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.73877 HOMO: -6.60965 LUMO: 2.38100 factor:1 | 1 (-0.10033) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.13905 HOMO: -6.73210 LUMO: 2.26127 factor:1 | 1 (-0.50061) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19685 HOMO: -6.76203 LUMO: 2.13609 factor:1 | 1 (-0.55840) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16787 HOMO: -6.71033 LUMO: 2.05990 factor:1 | 1 (-0.52942) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.46178 HOMO: -6.50896 LUMO: 2.32385 factor:1 | 1 (-0.82333) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25873 HOMO: -6.53345 LUMO: 1.74425 factor:1 | 1 (-0.62028) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17415 HOMO: -6.25862 LUMO: 1.63540 factor:1 | 1 (-0.53571) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14071 HOMO: -5.90759 LUMO: 1.78779 factor:1 | 1 (-0.50227) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.95148 HOMO: -6.09807 LUMO: 1.99732 factor:1 | 1 (-0.31304) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01083 HOMO: -5.92392 LUMO: 1.99732 factor:1 | 1 (-0.37239) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.00787 HOMO: -6.45182 LUMO: 1.72248 factor:1 | 1 (-0.36942) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19168 HOMO: -6.53073 LUMO: 1.82588 factor:1 | 1 (-0.55323) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.23791 HOMO: -6.40828 LUMO: 2.05174 factor:1 | 1 (-0.59947) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04798 HOMO: -6.60420 LUMO: -0.82450 factor:1 | 1 (-0.40953) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17467 HOMO: -6.76747 LUMO: -0.57144 factor:1 | 1 (-0.53623) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.24763 HOMO: -6.67767 LUMO: -0.59321 factor:1 | 1 (-0.60918) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02925 HOMO: -6.65863 LUMO: -0.57416 factor:1 | 1 (-0.39081) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.13630 HOMO: -6.49808 LUMO: -0.54695 factor:1 | 1 (-0.49786) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.90547 HOMO: -6.50080 LUMO: -0.61498 factor:1 | 1 (-0.26703) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.12403 HOMO: -6.74842 LUMO: -0.51974 factor:1 | 1 (-0.48559) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92683 HOMO: -6.13345 LUMO: 0.67756 factor:1 | 1 (-0.28839) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01540 HOMO: -6.48719 LUMO: 0.52790 factor:1 | 1 (-0.37696) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.85159 HOMO: -6.35930 LUMO: 0.74015 factor:1 | 1 (-0.21315) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04866 HOMO: -6.41644 LUMO: 0.22313 factor:1 | 1 (-0.41021) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.86686 HOMO: -6.85727 LUMO: -0.00272 factor:1 | 1 (-0.22841) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.81072 HOMO: -6.84638 LUMO: 0.24762 factor:1 | 1 (-0.17228) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.66941 HOMO: -6.66951 LUMO: 0.39184 factor:1 | 1 (-0.03097) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.12479 HOMO: -6.62597 LUMO: -0.65035 factor:1 | 1 (-0.48635) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92645 HOMO: -7.13755 LUMO: 0.45715 factor:1 | 1 (-0.28801) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.71687 HOMO: -7.12666 LUMO: 0.45171 factor:1 | 1 (-0.07842) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02000 HOMO: -6.46270 LUMO: -0.46259 factor:1 | 1 (-0.38156) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.82326 HOMO: -6.36202 LUMO: -0.29660 factor:1 | 1 (-0.18482) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.18474 HOMO: -6.28583 LUMO: 0.40545 factor:1 | 1 (-0.54630) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02425 HOMO: -6.70761 LUMO: 0.41906 factor:1 | 1 (-0.38580) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.18354 HOMO: -6.76203 LUMO: -0.60954 factor:1 | 1 (-0.54510) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.11456 HOMO: -6.85999 LUMO: -0.75103 factor:1 | 1 (-0.47612) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.73349 HOMO: -7.19741 LUMO: -1.00954 factor:1 | 1 (-0.09505) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14166 HOMO: -6.58243 LUMO: -0.33470 factor:1 | 1 (-0.50322) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09179 HOMO: -7.22190 LUMO: 0.49253 factor:1 | 1 (-0.45334) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.30305 HOMO: -7.22462 LUMO: 0.51974 factor:1 | 1 (-0.66461) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.37024 HOMO: -7.08584 LUMO: -0.68301 factor:1 | 1 (-0.73180) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25579 HOMO: -6.68584 LUMO: -0.29660 factor:1 | 1 (-0.61734) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.10471 HOMO: -6.33753 LUMO: -0.48436 factor:1 | 1 (-0.46627) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.88337 HOMO: -7.15932 LUMO: 0.55511 factor:1 | 1 (-0.24493) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.08047 HOMO: -6.57427 LUMO: 2.01908 factor:1 | 1 (-0.44202) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.08572 HOMO: -6.75659 LUMO: 2.22045 factor:1 | 1 (-0.44727) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09391 HOMO: -6.73482 LUMO: 2.20956 factor:1 | 1 (-0.45546) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.88343 HOMO: -6.74026 LUMO: 1.76602 factor:1 | 1 (-0.24498) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.24303 HOMO: -6.95523 LUMO: 1.94834 factor:1 | 1 (-0.60458) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.03940 HOMO: -6.33209 LUMO: 1.87486 factor:1 | 1 (-0.40096) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.32017 HOMO: -6.71033 LUMO: 2.12521 factor:1 | 1 (-0.68173) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17837 HOMO: -6.50080 LUMO: 2.04902 factor:1 | 1 (-0.53993) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04196 HOMO: -6.76475 LUMO: 1.94017 factor:1 | 1 (-0.40352) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.90405 HOMO: -6.53073 LUMO: 2.08983 factor:1 | 1 (-0.26561) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17426 HOMO: -6.69944 LUMO: 2.20684 factor:1 | 1 (-0.53582) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02716 HOMO: -6.34570 LUMO: 1.80684 factor:1 | 1 (-0.38871) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.93080 HOMO: -6.78380 LUMO: 1.95922 factor:1 | 1 (-0.29236) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19622 HOMO: -6.93618 LUMO: 1.76058 factor:1 | 1 (-0.55778) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.97954 HOMO: -6.93346 LUMO: 1.79595 factor:1 | 1 (-0.34109) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87916 HOMO: -6.29671 LUMO: 1.75241 factor:1 | 1 (-0.24071) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.78416 HOMO: -6.77019 LUMO: 1.74697 factor:1 | 1 (-0.14572) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.08776 HOMO: -6.87360 LUMO: 1.91024 factor:1 | 1 (-0.44931) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04112 HOMO: -6.32665 LUMO: 1.87759 factor:1 | 1 (-0.40267) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.12063 HOMO: -6.99877 LUMO: 1.99187 factor:1 | 1 (-0.48219) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.24077 HOMO: -6.72665 LUMO: 2.12521 factor:1 | 1 (-0.60232) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16909 HOMO: -6.67767 LUMO: 2.43814 factor:1 | 1 (-0.53065) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.18188 HOMO: -6.99605 LUMO: 1.79051 factor:1 | 1 (-0.54344) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.18934 HOMO: -6.25046 LUMO: 1.77146 factor:1 | 1 (-0.55089) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.03078 HOMO: -6.30488 LUMO: 1.90480 factor:1 | 1 (-0.39233) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04847 HOMO: -6.38379 LUMO: 1.68438 factor:1 | 1 (-0.41002) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.89839 HOMO: -6.78924 LUMO: 2.01364 factor:1 | 1 (-0.25995) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.82857 HOMO: -6.15249 LUMO: 1.98643 factor:1 | 1 (-0.19013) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09902 HOMO: -6.19331 LUMO: 2.14154 factor:1 | 1 (-0.46058) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.99665 HOMO: -6.05998 LUMO: 2.12521 factor:1 | 1 (-0.35821) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.78813 HOMO: -6.67223 LUMO: 1.91840 factor:1 | 1 (-0.14969) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02357 HOMO: -6.79196 LUMO: 2.18507 factor:1 | 1 (-0.38512) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.80661 HOMO: -6.93346 LUMO: 1.78235 factor:1 | 1 (-0.16817) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.93714 HOMO: -6.16882 LUMO: 1.80956 factor:1 | 1 (-0.29870) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02183 HOMO: -6.72665 LUMO: 2.07895 factor:1 | 1 (-0.38338) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.83499 HOMO: -6.73210 LUMO: 1.97827 factor:1 | 1 (-0.19655) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.96229 HOMO: -6.84638 LUMO: 1.87214 factor:1 | 1 (-0.32384) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87624 HOMO: -6.83006 LUMO: 2.36195 factor:1 | 1 (-0.23780) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.68196 HOMO: -6.97700 LUMO: 1.91024 factor:1 | 1 (-0.04351) | -1 | -1 |
| G: -5345.27275 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.06613 HOMO: -6.20420 LUMO: 1.81772 factor:1 | 1 (-0.42768) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.46015 HOMO: -7.09129 LUMO: 2.10344 factor:1 | 1 (-0.84853) | 1 | 1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.39288 HOMO: -6.77564 LUMO: 2.14970 factor:1 | 1 (-0.78127) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19614 HOMO: -6.81645 LUMO: 1.85854 factor:1 | 1 (-0.58453) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.32518 HOMO: -6.50896 LUMO: 2.04358 factor:1 | 1 (-0.71356) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.40232 HOMO: -6.89264 LUMO: 1.66262 factor:1 | 1 (-0.79071) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.22809 HOMO: -6.75931 LUMO: 2.23950 factor:1 | 1 (-0.61647) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.44472 HOMO: -6.50080 LUMO: 1.67622 factor:1 | 1 (-0.83310) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.33541 HOMO: -6.30216 LUMO: 2.24222 factor:1 | 1 (-0.72380) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.33829 HOMO: -7.18108 LUMO: 2.10072 factor:1 | 1 (-0.72668) | 1 | 1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.46793 HOMO: -6.54162 LUMO: 2.35378 factor:1 | 1 (-0.85632) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.37819 HOMO: -5.98650 LUMO: 1.48302 factor:1 | 1 (-0.76657) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.48050 HOMO: -7.15115 LUMO: 2.14970 factor:1 | 1 (-0.86889) | 1 | 1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.27761 HOMO: -6.45454 LUMO: 2.15786 factor:1 | 1 (-0.66600) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.20224 HOMO: -7.06952 LUMO: 2.14970 factor:1 | 1 (-0.59062) | 1 | 1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.41351 HOMO: -6.93618 LUMO: 1.86942 factor:1 | 1 (-0.80189) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.28352 HOMO: -6.63141 LUMO: 1.92657 factor:1 | 1 (-0.67190) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.03230 HOMO: -6.51441 LUMO: -0.44355 factor:1 | 1 (-0.42069) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.15867 HOMO: -6.82734 LUMO: -1.03131 factor:1 | 1 (-0.54706) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.03559 HOMO: -6.58788 LUMO: -0.82995 factor:1 | 1 (-0.42398) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19018 HOMO: -6.43277 LUMO: -0.40817 factor:1 | 1 (-0.57857) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.08047 HOMO: -6.78924 LUMO: -0.72110 factor:1 | 1 (-0.46885) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.34978 HOMO: -7.28177 LUMO: 0.36735 factor:1 | 1 (-0.73816) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16871 HOMO: -6.47903 LUMO: -0.46259 factor:1 | 1 (-0.55710) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.32183 HOMO: -6.67495 LUMO: -0.75376 factor:1 | 1 (-0.71022) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19024 HOMO: -6.71033 LUMO: -0.71838 factor:1 | 1 (-0.57862) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14953 HOMO: -6.79740 LUMO: -0.79185 factor:1 | 1 (-0.53791) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.49574 HOMO: -6.08719 LUMO: -0.63675 factor:1 | 1 (-0.88413) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19609 HOMO: -6.84094 LUMO: 0.42994 factor:1 | 1 (-0.58447) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.86596 HOMO: -6.59604 LUMO: 0.25851 factor:1 | 1 (-0.25434) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.05053 HOMO: -6.82462 LUMO: 0.08708 factor:1 | 1 (-0.43892) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.08131 HOMO: -6.54706 LUMO: 0.44082 factor:1 | 1 (-0.46970) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.29005 HOMO: -6.99333 LUMO: 0.32109 factor:1 | 1 (-0.67843) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14599 HOMO: -6.29944 LUMO: -0.57144 factor:1 | 1 (-0.53438) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92182 HOMO: -6.57699 LUMO: -0.46531 factor:1 | 1 (-0.31021) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.89121 HOMO: -6.24773 LUMO: -0.53879 factor:1 | 1 (-0.27960) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.11658 HOMO: -6.96067 LUMO: -0.67212 factor:1 | 1 (-0.50496) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17854 HOMO: -7.24095 LUMO: -0.09252 factor:1 | 1 (-0.56692) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09864 HOMO: -6.33481 LUMO: -0.46531 factor:1 | 1 (-0.48703) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25282 HOMO: -6.43549 LUMO: -0.33198 factor:1 | 1 (-0.64121) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17445 HOMO: -6.53073 LUMO: 0.44899 factor:1 | 1 (-0.56284) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.06705 HOMO: -6.69128 LUMO: 0.47620 factor:1 | 1 (-0.45544) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.38050 HOMO: -6.65318 LUMO: 0.52246 factor:1 | 1 (-0.76888) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.81532 HOMO: -6.71305 LUMO: 0.41089 factor:1 | 1 (-0.20370) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.86971 HOMO: -6.70216 LUMO: 0.19864 factor:1 | 1 (-0.25810) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.82174 HOMO: -6.41100 LUMO: 0.34558 factor:1 | 1 (-0.21013) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17728 HOMO: -7.01237 LUMO: 0.02993 factor:1 | 1 (-0.56567) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16615 HOMO: -6.85999 LUMO: 0.18776 factor:1 | 1 (-0.55454) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.11524 HOMO: -6.62869 LUMO: 0.48708 factor:1 | 1 (-0.50363) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.37451 HOMO: -6.43821 LUMO: -0.45715 factor:1 | 1 (-0.76290) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.28776 HOMO: -6.43277 LUMO: -0.72110 factor:1 | 1 (-0.67615) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.34627 HOMO: -7.10761 LUMO: 0.43266 factor:1 | 1 (-0.73465) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01929 HOMO: -6.57699 LUMO: -0.61498 factor:1 | 1 (-0.40768) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14224 HOMO: -6.82189 LUMO: -0.75648 factor:1 | 1 (-0.53062) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01021 HOMO: -6.55794 LUMO: -0.67212 factor:1 | 1 (-0.39859) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87540 HOMO: -6.69128 LUMO: 1.88575 factor:1 | 1 (-0.26379) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16009 HOMO: -6.65591 LUMO: 1.70888 factor:1 | 1 (-0.54847) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.95641 HOMO: -6.58788 LUMO: 1.68438 factor:1 | 1 (-0.34480) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.97616 HOMO: -6.46270 LUMO: 1.72520 factor:1 | 1 (-0.36455) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.11252 HOMO: -6.57427 LUMO: 1.73881 factor:1 | 1 (-0.50091) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.11723 HOMO: -6.45182 LUMO: 1.75241 factor:1 | 1 (-0.50561) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87488 HOMO: -6.51441 LUMO: 1.78779 factor:1 | 1 (-0.26327) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.71496 HOMO: -6.67495 LUMO: 2.11705 factor:1 | 1 (-0.10335) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25609 HOMO: -6.22597 LUMO: 1.96466 factor:1 | 1 (-0.64447) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.26847 HOMO: -6.68040 LUMO: 2.30753 factor:1 | 1 (-0.65686) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25726 HOMO: -6.65046 LUMO: 2.18235 factor:1 | 1 (-0.64564) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.55950 HOMO: -6.38651 LUMO: 1.76874 factor:1 | 1 (-0.94788) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.27750 HOMO: -6.41644 LUMO: 2.09256 factor:1 | 1 (-0.66589) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.05668 HOMO: -6.14977 LUMO: 2.28031 factor:1 | 1 (-0.44507) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.28020 HOMO: -6.70489 LUMO: 2.43814 factor:1 | 1 (-0.66858) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25345 HOMO: -6.78924 LUMO: 2.27215 factor:1 | 1 (-0.64183) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.24047 HOMO: -6.86271 LUMO: 2.31025 factor:1 | 1 (-0.62886) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.15372 HOMO: -6.51168 LUMO: 2.04630 factor:1 | 1 (-0.54211) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.50673 HOMO: -6.72665 LUMO: 2.13337 factor:1 | 1 (-0.89512) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.96751 HOMO: -6.45998 LUMO: 2.16058 factor:1 | 1 (-0.35590) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.84860 HOMO: -6.83822 LUMO: 2.20684 factor:1 | 1 (-0.23698) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.30618 HOMO: -6.68856 LUMO: 2.19324 factor:1 | 1 (-0.69457) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.20618 HOMO: -6.71577 LUMO: 2.16058 factor:1 | 1 (-0.59457) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.13051 HOMO: -6.82462 LUMO: 1.90208 factor:1 | 1 (-0.51889) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.23707 HOMO: -6.61509 LUMO: 2.23950 factor:1 | 1 (-0.62545) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.26311 HOMO: -6.73754 LUMO: 1.84221 factor:1 | 1 (-0.65150) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.41620 HOMO: -6.56611 LUMO: 1.94561 factor:1 | 1 (-0.80459) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.26063 HOMO: -6.67767 LUMO: 1.51840 factor:1 | 1 (-0.64902) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.15424 HOMO: -6.35658 LUMO: 2.16603 factor:1 | 1 (-0.54262) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.99440 HOMO: -6.35114 LUMO: 2.08983 factor:1 | 1 (-0.38278) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92346 HOMO: -6.35114 LUMO: 2.10616 factor:1 | 1 (-0.31184) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.88335 HOMO: -6.71305 LUMO: 2.01636 factor:1 | 1 (-0.27173) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.78201 HOMO: -6.24773 LUMO: 1.98915 factor:1 | 1 (-0.17040) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.15486 HOMO: -6.53617 LUMO: 2.42726 factor:1 | 1 (-0.54325) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.10692 HOMO: -6.59332 LUMO: 1.82316 factor:1 | 1 (-0.49530) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92781 HOMO: -6.41372 LUMO: 1.77418 factor:1 | 1 (-0.31620) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.13135 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-0.51974) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09598 HOMO: -6.11168 LUMO: 1.70888 factor:1 | 1 (-0.48436) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.12313 HOMO: -6.44910 LUMO: 2.23405 factor:1 | 1 (-0.51152) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25592 HOMO: -6.24773 LUMO: 2.12793 factor:1 | 1 (-0.64431) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02115 HOMO: -6.07358 LUMO: 1.89663 factor:1 | 1 (-0.40953) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14732 HOMO: -6.66679 LUMO: 1.96738 factor:1 | 1 (-0.53571) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.03222 HOMO: -6.68312 LUMO: 1.78235 factor:1 | 1 (-0.42061) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.46102 HOMO: -6.70761 LUMO: 1.97555 factor:1 | 1 (-0.84940) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.22452 HOMO: -6.15794 LUMO: 2.00548 factor:1 | 1 (-0.61291) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.97997 HOMO: -6.52257 LUMO: 1.96738 factor:1 | 1 (-0.36836) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09211 HOMO: -6.25590 LUMO: 1.86670 factor:1 | 1 (-0.48050) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92218 HOMO: -6.30216 LUMO: 1.84765 factor:1 | 1 (-0.31056) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.24069 HOMO: -6.76747 LUMO: 2.20956 factor:1 | 1 (-0.62907) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17103 HOMO: -6.14161 LUMO: 1.80684 factor:1 | 1 (-0.55941) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09023 HOMO: -6.81373 LUMO: 1.91024 factor:1 | 1 (-0.47862) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.96008 HOMO: -6.81917 LUMO: 2.34834 factor:1 | 1 (-0.34847) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.82209 HOMO: -6.72121 LUMO: 1.90208 factor:1 | 1 (-0.21048) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.70702 HOMO: -7.51851 LUMO: 0.26939 factor:1 | 1 (-0.09540) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87921 HOMO: -6.65318 LUMO: -0.57144 factor:1 | 1 (-0.26760) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.93298 HOMO: -6.77564 LUMO: -0.72654 factor:1 | 1 (-0.32137) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87023 HOMO: -6.80557 LUMO: -0.60954 factor:1 | 1 (-0.25862) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.72898 HOMO: -7.35524 LUMO: 0.27483 factor:1 | 1 (-0.11736) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.15573 HOMO: -6.94979 LUMO: -0.83811 factor:1 | 1 (-0.54412) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09238 HOMO: -6.13345 LUMO: -0.67212 factor:1 | 1 (-0.48077) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.06384 HOMO: -6.47359 LUMO: -0.59321 factor:1 | 1 (-0.45223) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.86680 HOMO: -6.52257 LUMO: -0.54695 factor:1 | 1 (-0.25519) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.32458 HOMO: -6.61781 LUMO: -0.69661 factor:1 | 1 (-0.71297) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14493 HOMO: -6.77564 LUMO: -0.80001 factor:1 | 1 (-0.53332) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16504 HOMO: -7.35252 LUMO: -1.00410 factor:1 | 1 (-0.55343) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16931 HOMO: -6.35386 LUMO: -0.38912 factor:1 | 1 (-0.55770) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.43917 HOMO: -6.80285 LUMO: -0.52246 factor:1 | 1 (-0.82755) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.32082 HOMO: -7.23279 LUMO: 0.30477 factor:1 | 1 (-0.70921) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04438 HOMO: -7.13483 LUMO: -0.76192 factor:1 | 1 (-0.43277) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.90727 HOMO: -6.71849 LUMO: -0.48164 factor:1 | 1 (-0.29565) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92781 HOMO: -6.85455 LUMO: -0.69389 factor:1 | 1 (-0.31620) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.15992 HOMO: -6.96339 LUMO: -0.73743 factor:1 | 1 (-0.54831) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.91513 HOMO: -7.50490 LUMO: 0.28844 factor:1 | 1 (-0.30352) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14077 HOMO: -6.63958 LUMO: -0.50069 factor:1 | 1 (-0.52915) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01617 HOMO: -6.78924 LUMO: -0.69661 factor:1 | 1 (-0.40455) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.23979 HOMO: -7.44776 LUMO: 0.33742 factor:1 | 1 (-0.62817) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.21674 HOMO: -6.15249 LUMO: 0.66396 factor:1 | 1 (-0.60513) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17590 HOMO: -6.17426 LUMO: 0.55511 factor:1 | 1 (-0.56428) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.38063 HOMO: -6.83550 LUMO: 0.28844 factor:1 | 1 (-0.76902) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.05679 HOMO: -6.32393 LUMO: 0.47620 factor:1 | 1 (-0.44518) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.99641 HOMO: -6.32937 LUMO: 0.45987 factor:1 | 1 (-0.38480) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.32379 HOMO: -7.37429 LUMO: 0.09252 factor:1 | 1 (-0.71218) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.86724 HOMO: -6.54434 LUMO: -0.39729 factor:1 | 1 (-0.25562) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.79698 HOMO: -7.35524 LUMO: 0.28028 factor:1 | 1 (-0.18536) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.71689 HOMO: -6.95523 LUMO: -0.86804 factor:1 | 1 (-0.10528) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.23720 HOMO: -6.63958 LUMO: -0.65307 factor:1 | 1 (-0.62559) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.20458 HOMO: -6.73482 LUMO: -0.67212 factor:1 | 1 (-0.59296) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.18972 HOMO: -6.37835 LUMO: -0.53606 factor:1 | 1 (-0.57811) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.39903 HOMO: -6.71849 LUMO: -0.61226 factor:1 | 1 (-0.78742) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04860 HOMO: -6.68584 LUMO: -1.11022 factor:1 | 1 (-0.43699) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04817 HOMO: -6.80285 LUMO: -0.79185 factor:1 | 1 (-0.43655) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.97418 HOMO: -7.14571 LUMO: -0.94696 factor:1 | 1 (-0.36256) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01423 HOMO: -7.16204 LUMO: -0.66124 factor:1 | 1 (-0.40262) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.88128 HOMO: -6.54978 LUMO: -0.54967 factor:1 | 1 (-0.26966) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.08267 HOMO: -6.75114 LUMO: -0.70750 factor:1 | 1 (-0.47106) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.95831 HOMO: -7.22190 LUMO: 0.39184 factor:1 | 1 (-0.34670) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14996 HOMO: -7.43959 LUMO: 0.30477 factor:1 | 1 (-0.53835) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.12879 HOMO: -6.87360 LUMO: -0.77552 factor:1 | 1 (-0.51718) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.20569 HOMO: -6.82734 LUMO: -0.59593 factor:1 | 1 (-0.59408) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16332 HOMO: -6.65318 LUMO: -0.46259 factor:1 | 1 (-0.55171) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87333 HOMO: -7.05863 LUMO: -1.17009 factor:1 | 1 (-0.26172) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.82492 HOMO: -6.57427 LUMO: -0.48708 factor:1 | 1 (-0.21331) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.70122 HOMO: -6.60420 LUMO: -0.38096 factor:1 | 1 (-0.08961) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.95222 HOMO: -6.72121 LUMO: -0.66668 factor:1 | 1 (-0.34060) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.81992 HOMO: -6.52257 LUMO: -0.19320 factor:1 | 1 (-0.20830) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.63292 HOMO: -6.28039 LUMO: -0.27211 factor:1 | 1 (-0.02131) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.90495 HOMO: -6.71849 LUMO: -0.42722 factor:1 | 1 (-0.29334) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01562 HOMO: -6.27495 LUMO: 0.27756 factor:1 | 1 (-0.40401) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.96452 HOMO: -6.21780 LUMO: 0.46531 factor:1 | 1 (-0.35290) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.18221 HOMO: -6.52257 LUMO: -0.64491 factor:1 | 1 (-0.57060) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.75333 HOMO: -6.73754 LUMO: 1.83133 factor:1 | 1 (-0.14172) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.00743 HOMO: -6.67223 LUMO: 1.88847 factor:1 | 1 (-0.39582) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.90416 HOMO: -6.82189 LUMO: 1.59187 factor:1 | 1 (-0.29255) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.03804 HOMO: -6.43277 LUMO: 1.76330 factor:1 | 1 (-0.42643) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16414 HOMO: -6.48175 LUMO: 1.77962 factor:1 | 1 (-0.55253) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.24741 HOMO: -6.50352 LUMO: 1.68438 factor:1 | 1 (-0.63579) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.05489 HOMO: -6.31576 LUMO: 2.03813 factor:1 | 1 (-0.44327) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.37337 HOMO: -6.27495 LUMO: 1.99459 factor:1 | 1 (-0.76176) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.13470 HOMO: -6.23957 LUMO: 2.17147 factor:1 | 1 (-0.52308) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.05238 HOMO: -6.78108 LUMO: 2.16875 factor:1 | 1 (-0.44077) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.93488 HOMO: -6.34297 LUMO: 2.10344 factor:1 | 1 (-0.32327) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.31906 HOMO: -6.30216 LUMO: 2.00004 factor:1 | 1 (-0.70744) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92688 HOMO: -6.72665 LUMO: 2.09528 factor:1 | 1 (-0.31527) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.84351 HOMO: -6.86543 LUMO: 1.91568 factor:1 | 1 (-0.23190) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.73877 HOMO: -5.83956 LUMO: 1.89391 factor:1 | 1 (-0.12716) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.13905 HOMO: -6.42189 LUMO: 2.03269 factor:1 | 1 (-0.52744) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19685 HOMO: -6.07630 LUMO: 1.80956 factor:1 | 1 (-0.58524) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16787 HOMO: -6.43277 LUMO: 1.81772 factor:1 | 1 (-0.55626) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.46178 HOMO: -7.03959 LUMO: 1.78779 factor:1 | 1 (-0.85017) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25873 HOMO: -6.72121 LUMO: 2.29664 factor:1 | 1 (-0.64711) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17415 HOMO: -6.62869 LUMO: 2.04630 factor:1 | 1 (-0.56254) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14071 HOMO: -6.63958 LUMO: 1.84221 factor:1 | 1 (-0.52910) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.95148 HOMO: -6.70761 LUMO: 1.67350 factor:1 | 1 (-0.33987) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01083 HOMO: -6.00283 LUMO: 1.64357 factor:1 | 1 (-0.39922) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.00787 HOMO: -6.48719 LUMO: 1.70343 factor:1 | 1 (-0.39625) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19168 HOMO: -6.13345 LUMO: 1.44492 factor:1 | 1 (-0.58007) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.23791 HOMO: -6.11168 LUMO: 1.70071 factor:1 | 1 (-0.62630) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04798 HOMO: -6.09535 LUMO: 1.82316 factor:1 | 1 (-0.43636) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17467 HOMO: -6.81101 LUMO: 1.63540 factor:1 | 1 (-0.56306) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.24763 HOMO: -6.80013 LUMO: 2.12249 factor:1 | 1 (-0.63601) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02925 HOMO: -6.48447 LUMO: 1.94561 factor:1 | 1 (-0.41764) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.13630 HOMO: -6.72393 LUMO: 2.06534 factor:1 | 1 (-0.52469) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.90547 HOMO: -6.34570 LUMO: 1.98915 factor:1 | 1 (-0.29386) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.12403 HOMO: -6.31304 LUMO: 1.87759 factor:1 | 1 (-0.51242) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92683 HOMO: -6.77564 LUMO: 1.81228 factor:1 | 1 (-0.31522) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01540 HOMO: -6.58516 LUMO: 2.34834 factor:1 | 1 (-0.40379) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.85159 HOMO: -6.68040 LUMO: 2.20412 factor:1 | 1 (-0.23998) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04866 HOMO: -6.20964 LUMO: 2.17147 factor:1 | 1 (-0.43704) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.86686 HOMO: -6.54706 LUMO: 2.03813 factor:1 | 1 (-0.25524) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.81072 HOMO: -6.54162 LUMO: 2.17419 factor:1 | 1 (-0.19911) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.66941 HOMO: -6.75659 LUMO: 2.22589 factor:1 | 1 (-0.05780) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.12479 HOMO: -6.59604 LUMO: 2.59325 factor:1 | 1 (-0.51318) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92645 HOMO: -6.11712 LUMO: 2.02181 factor:1 | 1 (-0.31484) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.71687 HOMO: -6.63141 LUMO: 2.09256 factor:1 | 1 (-0.10525) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02000 HOMO: -6.61781 LUMO: 1.86126 factor:1 | 1 (-0.40839) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.82326 HOMO: -6.63958 LUMO: 1.77146 factor:1 | 1 (-0.21165) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.18474 HOMO: -6.60420 LUMO: 1.54561 factor:1 | 1 (-0.57313) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02425 HOMO: -6.52529 LUMO: 2.05174 factor:1 | 1 (-0.41263) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.18354 HOMO: -6.80285 LUMO: 2.13609 factor:1 | 1 (-0.57193) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.11456 HOMO: -6.51168 LUMO: 2.25855 factor:1 | 1 (-0.50295) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.73349 HOMO: -6.64774 LUMO: 2.46263 factor:1 | 1 (-0.12188) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14166 HOMO: -6.40828 LUMO: 1.99732 factor:1 | 1 (-0.53005) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09179 HOMO: -5.97562 LUMO: 1.56465 factor:1 | 1 (-0.48017) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.30305 HOMO: -6.75659 LUMO: 2.23405 factor:1 | 1 (-0.69144) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.37024 HOMO: -6.68584 LUMO: 2.09528 factor:1 | 1 (-0.75863) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25579 HOMO: -6.86543 LUMO: 1.95106 factor:1 | 1 (-0.64418) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.10471 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-0.49310) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.88337 HOMO: -6.87632 LUMO: 2.08439 factor:1 | 1 (-0.27176) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.08047 HOMO: -6.33753 LUMO: 2.16603 factor:1 | 1 (-0.46885) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.08572 HOMO: -6.92258 LUMO: 1.72248 factor:1 | 1 (-0.47410) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09391 HOMO: -6.62597 LUMO: 2.10344 factor:1 | 1 (-0.48229) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.88343 HOMO: -6.63141 LUMO: 1.94017 factor:1 | 1 (-0.27181) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.24303 HOMO: -6.48447 LUMO: 1.91840 factor:1 | 1 (-0.63141) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.03940 HOMO: -6.41372 LUMO: 1.61364 factor:1 | 1 (-0.42779) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.32017 HOMO: -6.37291 LUMO: 1.79051 factor:1 | 1 (-0.70856) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17837 HOMO: -6.13073 LUMO: 1.77962 factor:1 | 1 (-0.56676) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04196 HOMO: -6.13073 LUMO: 1.98915 factor:1 | 1 (-0.43035) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.90405 HOMO: -6.44094 LUMO: 1.58370 factor:1 | 1 (-0.29244) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17426 HOMO: -6.87087 LUMO: -0.82995 factor:1 | 1 (-0.56265) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02716 HOMO: -6.67223 LUMO: 1.08029 factor:1 | 1 (-0.41555) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.93080 HOMO: -6.82462 LUMO: 0.91702 factor:1 | 1 (-0.31919) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19622 HOMO: -6.65863 LUMO: 1.52656 factor:1 | 1 (-0.58461) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.97954 HOMO: -6.78924 LUMO: 0.86260 factor:1 | 1 (-0.36793) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87916 HOMO: -6.68584 LUMO: 0.94424 factor:1 | 1 (-0.26754) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.78416 HOMO: -6.58788 LUMO: 1.00138 factor:1 | 1 (-0.17255) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.08776 HOMO: -6.79740 LUMO: 0.91430 factor:1 | 1 (-0.47614) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04112 HOMO: -6.67223 LUMO: 0.80274 factor:1 | 1 (-0.42950) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.12063 HOMO: -6.95251 LUMO: 0.90614 factor:1 | 1 (-0.50902) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.24077 HOMO: -7.19469 LUMO: 1.34152 factor:1 | 1 (-0.62915) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16909 HOMO: -6.59332 LUMO: -0.76464 factor:1 | 1 (-0.55748) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.18188 HOMO: -6.77564 LUMO: -0.90886 factor:1 | 1 (-0.57027) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.18934 HOMO: -6.57971 LUMO: -0.41633 factor:1 | 1 (-0.57772) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.03078 HOMO: -6.68856 LUMO: -0.58232 factor:1 | 1 (-0.41916) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04847 HOMO: -6.87087 LUMO: -0.71022 factor:1 | 1 (-0.43685) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.89839 HOMO: -6.67767 LUMO: -0.74559 factor:1 | 1 (-0.28678) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.82857 HOMO: -6.68040 LUMO: -0.65307 factor:1 | 1 (-0.21696) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09902 HOMO: -6.32937 LUMO: 0.80274 factor:1 | 1 (-0.48741) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.99665 HOMO: -6.29671 LUMO: 0.82723 factor:1 | 1 (-0.38504) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.78813 HOMO: -6.67767 LUMO: 0.59321 factor:1 | 1 (-0.17652) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02357 HOMO: -6.77836 LUMO: 0.50341 factor:1 | 1 (-0.41195) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.80661 HOMO: -6.61781 LUMO: 0.42450 factor:1 | 1 (-0.19500) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.93714 HOMO: -6.83278 LUMO: 0.39457 factor:1 | 1 (-0.32553) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02183 HOMO: -6.56883 LUMO: 0.64219 factor:1 | 1 (-0.41021) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.83499 HOMO: -6.71577 LUMO: 0.40001 factor:1 | 1 (-0.22338) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.96229 HOMO: -6.86543 LUMO: -0.74287 factor:1 | 1 (-0.35067) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87624 HOMO: -6.68584 LUMO: -0.69389 factor:1 | 1 (-0.26463) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.68196 HOMO: -6.61237 LUMO: -0.48980 factor:1 | 1 (-0.07034) | -1 | -1 |
| G: -5345.24592 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.06613 HOMO: -6.80285 LUMO: -0.58232 factor:1 | 1 (-0.45451) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.46015 HOMO: -6.88992 LUMO: -0.70205 factor:1 | 1 (-0.08574) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.39288 HOMO: -6.95251 LUMO: -0.71838 factor:1 | 1 (-0.01848) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19614 HOMO: -7.52123 LUMO: 0.27211 factor:1 | -1 (0.17826) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.32518 HOMO: -6.76747 LUMO: -0.74015 factor:1 | -1 (0.04923) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.40232 HOMO: -6.55250 LUMO: -0.49797 factor:1 | 1 (-0.02792) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.22809 HOMO: -6.50896 LUMO: -0.46804 factor:1 | -1 (0.14632) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.44472 HOMO: -7.45320 LUMO: 0.08436 factor:1 | 1 (-0.07031) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.33541 HOMO: -6.82462 LUMO: -0.70477 factor:1 | -1 (0.03899) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.33829 HOMO: -6.57155 LUMO: -0.43538 factor:1 | -1 (0.03611) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.46793 HOMO: -6.72665 LUMO: -0.55239 factor:1 | 1 (-0.09353) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.37819 HOMO: -7.05319 LUMO: -1.08573 factor:1 | 1 (-0.00378) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.48050 HOMO: -6.56067 LUMO: -0.45715 factor:1 | 1 (-0.10610) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.27761 HOMO: -6.76475 LUMO: -0.53879 factor:1 | -1 (0.09679) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.20224 HOMO: -6.67223 LUMO: -0.45987 factor:1 | -1 (0.17217) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.41351 HOMO: -6.44094 LUMO: -0.72110 factor:1 | 1 (-0.03910) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.28352 HOMO: -6.66951 LUMO: -0.67756 factor:1 | -1 (0.09089) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.03230 HOMO: -6.69400 LUMO: -0.62858 factor:1 | -1 (0.34210) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.15867 HOMO: -6.51985 LUMO: -0.37007 factor:1 | -1 (0.21573) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.03559 HOMO: -5.98378 LUMO: 0.78641 factor:1 | -1 (0.33881) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19018 HOMO: -6.11440 LUMO: 0.71294 factor:1 | -1 (0.18422) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.08047 HOMO: -6.45182 LUMO: 0.63947 factor:1 | -1 (0.29394) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.34978 HOMO: -6.78924 LUMO: 0.37007 factor:1 | -1 (0.02463) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16871 HOMO: -6.63686 LUMO: 0.54423 factor:1 | -1 (0.20569) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.32183 HOMO: -6.66679 LUMO: 0.48708 factor:1 | -1 (0.05257) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19024 HOMO: -6.81917 LUMO: 0.31021 factor:1 | -1 (0.18417) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14953 HOMO: -6.28583 LUMO: 0.44899 factor:1 | -1 (0.22487) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.49574 HOMO: -6.61237 LUMO: 0.49525 factor:1 | 1 (-0.12134) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19609 HOMO: -7.08857 LUMO: 0.38368 factor:1 | -1 (0.17832) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.86596 HOMO: -6.53890 LUMO: -0.68845 factor:1 | -1 (0.50844) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.05053 HOMO: -6.56611 LUMO: -0.66396 factor:1 | -1 (0.32387) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.08131 HOMO: -6.04909 LUMO: -0.59865 factor:1 | -1 (0.29309) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.29005 HOMO: -6.74842 LUMO: -0.77825 factor:1 | -1 (0.08436) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14599 HOMO: -6.82462 LUMO: -0.61498 factor:1 | -1 (0.22841) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92182 HOMO: -7.40694 LUMO: 0.32926 factor:1 | -1 (0.45258) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.89121 HOMO: -6.80557 LUMO: -0.57416 factor:1 | -1 (0.48319) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.11658 HOMO: -6.76747 LUMO: -0.67484 factor:1 | -1 (0.25783) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17854 HOMO: -7.23279 LUMO: 0.48980 factor:1 | -1 (0.19587) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09864 HOMO: -6.62869 LUMO: -0.24762 factor:1 | -1 (0.27576) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25282 HOMO: -6.65863 LUMO: -0.28028 factor:1 | -1 (0.12158) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17445 HOMO: -6.50352 LUMO: -0.44899 factor:1 | -1 (0.19995) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.06705 HOMO: -6.62053 LUMO: -0.88437 factor:1 | -1 (0.30735) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.38050 HOMO: -6.73754 LUMO: -0.77825 factor:1 | 1 (-0.00610) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.81532 HOMO: -7.24639 LUMO: 0.35647 factor:1 | -1 (0.55909) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.86971 HOMO: -6.46270 LUMO: -0.48164 factor:1 | -1 (0.50469) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.82174 HOMO: -6.14161 LUMO: -0.66396 factor:1 | -1 (0.55266) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17728 HOMO: -6.63414 LUMO: 1.51295 factor:1 | -1 (0.19712) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16615 HOMO: -6.52529 LUMO: 1.65989 factor:1 | -1 (0.20825) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.11524 HOMO: -6.63686 LUMO: 1.64629 factor:1 | -1 (0.25916) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.37451 HOMO: -6.49808 LUMO: 1.60003 factor:1 | 1 (-0.00011) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.28776 HOMO: -6.85183 LUMO: 1.96194 factor:1 | -1 (0.08664) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.34627 HOMO: -6.90081 LUMO: 1.82316 factor:1 | -1 (0.02814) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01929 HOMO: -6.20147 LUMO: 1.95106 factor:1 | -1 (0.35511) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14224 HOMO: -7.05047 LUMO: 1.94289 factor:1 | -1 (0.23217) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01021 HOMO: -6.11440 LUMO: 1.83949 factor:1 | -1 (0.36420) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87540 HOMO: -6.65046 LUMO: 1.59187 factor:1 | -1 (0.49900) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16009 HOMO: -6.81917 LUMO: 2.41365 factor:1 | -1 (0.21432) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.95641 HOMO: -6.40284 LUMO: 2.48984 factor:1 | -1 (0.41799) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.97616 HOMO: -7.04775 LUMO: 2.31025 factor:1 | -1 (0.39824) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.11252 HOMO: -6.64774 LUMO: 2.20140 factor:1 | -1 (0.26188) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.11723 HOMO: -6.72393 LUMO: 2.28304 factor:1 | -1 (0.25717) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87488 HOMO: -6.35114 LUMO: 1.84765 factor:1 | -1 (0.49952) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.71496 HOMO: -6.41100 LUMO: 1.74697 factor:1 | -1 (0.65944) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25609 HOMO: -6.34297 LUMO: 1.55921 factor:1 | -1 (0.11832) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.26847 HOMO: -6.31848 LUMO: 1.67622 factor:1 | -1 (0.10593) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25726 HOMO: -6.50896 LUMO: 2.02725 factor:1 | -1 (0.11715) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.55950 HOMO: -6.28583 LUMO: 2.00548 factor:1 | 1 (-0.18509) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.27750 HOMO: -6.67495 LUMO: 1.92384 factor:1 | -1 (0.09690) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.05668 HOMO: -6.17154 LUMO: 2.39732 factor:1 | -1 (0.31772) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.28020 HOMO: -6.84911 LUMO: 2.24766 factor:1 | -1 (0.09421) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25345 HOMO: -6.77564 LUMO: 2.38372 factor:1 | -1 (0.12095) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.24047 HOMO: -6.18243 LUMO: 2.40821 factor:1 | -1 (0.13393) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.15372 HOMO: -6.40828 LUMO: 2.22589 factor:1 | -1 (0.22068) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.50673 HOMO: -6.74570 LUMO: 1.88303 factor:1 | 1 (-0.13233) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.96751 HOMO: -6.29944 LUMO: 2.05174 factor:1 | -1 (0.40689) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.84860 HOMO: -7.00693 LUMO: 2.16331 factor:1 | -1 (0.52581) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.30618 HOMO: -6.89537 LUMO: 2.19596 factor:1 | -1 (0.06822) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.20618 HOMO: -6.72665 LUMO: 2.03813 factor:1 | -1 (0.16822) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.13051 HOMO: -6.69944 LUMO: 2.36467 factor:1 | -1 (0.24390) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.23707 HOMO: -6.92802 LUMO: 1.72792 factor:1 | -1 (0.13734) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.26311 HOMO: -6.12256 LUMO: 1.85310 factor:1 | -1 (0.11129) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.41620 HOMO: -6.70489 LUMO: 2.20956 factor:1 | 1 (-0.04180) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.26063 HOMO: -6.94707 LUMO: 1.81500 factor:1 | -1 (0.11377) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.15424 HOMO: -6.39468 LUMO: 1.79051 factor:1 | -1 (0.22017) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.99440 HOMO: -6.69128 LUMO: 2.03813 factor:1 | -1 (0.38001) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92346 HOMO: -6.55250 LUMO: 2.00548 factor:1 | -1 (0.45095) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.88335 HOMO: -6.24773 LUMO: 2.09256 factor:1 | -1 (0.49106) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.78201 HOMO: -6.85727 LUMO: 1.70071 factor:1 | -1 (0.59239) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.15486 HOMO: -6.71305 LUMO: 1.72520 factor:1 | -1 (0.21954) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.10692 HOMO: -6.81101 LUMO: 2.15514 factor:1 | -1 (0.26749) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92781 HOMO: -6.93618 LUMO: 1.75513 factor:1 | -1 (0.44659) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.13135 HOMO: -6.63686 LUMO: 2.09800 factor:1 | -1 (0.24305) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09598 HOMO: -6.98244 LUMO: 1.72520 factor:1 | -1 (0.27843) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.12313 HOMO: -6.37019 LUMO: 2.35923 factor:1 | -1 (0.25127) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25592 HOMO: -6.55794 LUMO: 2.12521 factor:1 | -1 (0.11848) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02115 HOMO: -6.45998 LUMO: 1.93201 factor:1 | -1 (0.35326) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14732 HOMO: -6.71033 LUMO: 1.58370 factor:1 | -1 (0.22708) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.03222 HOMO: -6.67223 LUMO: 1.52928 factor:1 | -1 (0.34218) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.46102 HOMO: -6.72121 LUMO: 1.33608 factor:1 | 1 (-0.08661) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.22452 HOMO: -6.89264 LUMO: 2.08983 factor:1 | -1 (0.14988) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.97997 HOMO: -6.31032 LUMO: 2.24766 factor:1 | -1 (0.39443) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09211 HOMO: -6.79740 LUMO: 2.09528 factor:1 | -1 (0.28229) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92218 HOMO: -6.78108 LUMO: 2.15786 factor:1 | -1 (0.45223) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.24069 HOMO: -6.50896 LUMO: 2.15786 factor:1 | -1 (0.13372) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17103 HOMO: -6.56067 LUMO: 2.24494 factor:1 | -1 (0.20338) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09023 HOMO: -6.72938 LUMO: 2.24494 factor:1 | -1 (0.28417) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.96008 HOMO: -6.40556 LUMO: 1.58642 factor:1 | -1 (0.41432) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.82209 HOMO: -6.63141 LUMO: 1.66262 factor:1 | -1 (0.55231) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.70702 HOMO: -6.97156 LUMO: 2.23678 factor:1 | -1 (0.66739) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87921 HOMO: -6.86271 LUMO: 1.91296 factor:1 | -1 (0.49519) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.93298 HOMO: -6.50624 LUMO: 1.89119 factor:1 | -1 (0.44142) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87023 HOMO: -6.70761 LUMO: 1.56193 factor:1 | -1 (0.50417) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.72898 HOMO: -6.60420 LUMO: 1.79595 factor:1 | -1 (0.64543) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.15573 HOMO: -6.85727 LUMO: 2.26943 factor:1 | -1 (0.21867) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09238 HOMO: -6.23413 LUMO: 1.91024 factor:1 | -1 (0.28202) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.06384 HOMO: -6.84366 LUMO: 2.01364 factor:1 | -1 (0.31056) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.86680 HOMO: -6.63414 LUMO: 2.54971 factor:1 | -1 (0.50760) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.32458 HOMO: -6.52257 LUMO: 2.42998 factor:1 | -1 (0.04982) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14493 HOMO: -6.61509 LUMO: 2.31297 factor:1 | -1 (0.22947) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16504 HOMO: -6.45998 LUMO: 2.23405 factor:1 | -1 (0.20936) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16931 HOMO: -6.86271 LUMO: 2.22317 factor:1 | -1 (0.20509) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.43917 HOMO: -6.84366 LUMO: 2.11432 factor:1 | 1 (-0.06476) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.32082 HOMO: -6.85999 LUMO: 2.44902 factor:1 | -1 (0.05358) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04438 HOMO: -6.73482 LUMO: 1.93745 factor:1 | -1 (0.33002) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.90727 HOMO: -6.91441 LUMO: 2.32385 factor:1 | -1 (0.46714) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92781 HOMO: -6.16066 LUMO: 2.26399 factor:1 | -1 (0.44659) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.15992 HOMO: -6.71305 LUMO: 2.38644 factor:1 | -1 (0.21448) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.91513 HOMO: -7.08312 LUMO: 2.01636 factor:1 | -1 (0.45927) | 1 | 1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14077 HOMO: -6.15249 LUMO: 1.90752 factor:1 | -1 (0.23364) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01617 HOMO: -6.83006 LUMO: 2.25855 factor:1 | -1 (0.35824) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.23979 HOMO: -6.77836 LUMO: 2.24766 factor:1 | -1 (0.13461) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.21674 HOMO: -6.66951 LUMO: 2.35923 factor:1 | -1 (0.15766) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17590 HOMO: -6.68312 LUMO: 2.30208 factor:1 | -1 (0.19851) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.38063 HOMO: -6.49808 LUMO: 2.49801 factor:1 | 1 (-0.00623) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.05679 HOMO: -6.62325 LUMO: 1.89935 factor:1 | -1 (0.31761) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.99641 HOMO: -6.80829 LUMO: 1.91296 factor:1 | -1 (0.37799) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.32379 HOMO: -6.64230 LUMO: 2.13065 factor:1 | -1 (0.05061) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.86724 HOMO: -6.40556 LUMO: 1.83949 factor:1 | -1 (0.50717) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.79698 HOMO: -6.48175 LUMO: 1.72248 factor:1 | -1 (0.57743) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.71689 HOMO: -6.61781 LUMO: 2.11432 factor:1 | -1 (0.65751) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.23720 HOMO: -6.34570 LUMO: 2.22317 factor:1 | -1 (0.13720) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.20458 HOMO: -7.00149 LUMO: 1.80139 factor:1 | -1 (0.16983) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.18972 HOMO: -6.66951 LUMO: 2.13065 factor:1 | -1 (0.18468) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.39903 HOMO: -6.54434 LUMO: 2.20140 factor:1 | 1 (-0.02463) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04860 HOMO: -6.67767 LUMO: 2.02997 factor:1 | -1 (0.32580) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04817 HOMO: -6.49536 LUMO: 2.42998 factor:1 | -1 (0.32624) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.97418 HOMO: -6.70761 LUMO: 2.71025 factor:1 | -1 (0.40023) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01423 HOMO: -6.62869 LUMO: 2.11160 factor:1 | -1 (0.36017) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.88128 HOMO: -6.61781 LUMO: 2.24494 factor:1 | -1 (0.49312) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.08267 HOMO: -6.66135 LUMO: 2.20956 factor:1 | -1 (0.29173) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.95831 HOMO: -6.95523 LUMO: 2.03813 factor:1 | -1 (0.41609) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14996 HOMO: -7.11578 LUMO: 2.41365 factor:1 | -1 (0.22444) | 1 | 1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.12879 HOMO: -6.99061 LUMO: 2.13881 factor:1 | -1 (0.24561) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.20569 HOMO: -6.43277 LUMO: 2.01364 factor:1 | -1 (0.16871) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16332 HOMO: -6.79196 LUMO: 2.04358 factor:1 | -1 (0.21108) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87333 HOMO: -7.08584 LUMO: 1.99732 factor:1 | -1 (0.50107) | 1 | 1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.82492 HOMO: -6.46815 LUMO: 2.29936 factor:1 | -1 (0.54948) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.70122 HOMO: -6.78108 LUMO: 1.93745 factor:1 | -1 (0.67318) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.95222 HOMO: -6.43277 LUMO: 1.80956 factor:1 | -1 (0.42218) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.81992 HOMO: -6.71577 LUMO: -0.81090 factor:1 | -1 (0.55449) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.63292 HOMO: -7.14027 LUMO: -0.68028 factor:1 | -1 (0.74148) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.90495 HOMO: -7.03414 LUMO: -0.69661 factor:1 | -1 (0.46945) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01562 HOMO: -6.64502 LUMO: -0.47348 factor:1 | -1 (0.35878) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.96452 HOMO: -6.60692 LUMO: 2.12793 factor:1 | -1 (0.40989) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.18221 HOMO: -6.66407 LUMO: 1.94561 factor:1 | -1 (0.19219) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.75333 HOMO: -7.10217 LUMO: 1.92384 factor:1 | -1 (0.62107) | 1 | 1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.00743 HOMO: -6.84094 LUMO: 1.66534 factor:1 | -1 (0.36697) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.90416 HOMO: -6.93618 LUMO: 2.13065 factor:1 | -1 (0.47024) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.03804 HOMO: -6.60692 LUMO: 2.20684 factor:1 | -1 (0.33636) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16414 HOMO: -6.85727 LUMO: 2.19324 factor:1 | -1 (0.21026) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.24741 HOMO: -6.31032 LUMO: 1.76330 factor:1 | -1 (0.12700) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.05489 HOMO: -6.43821 LUMO: 2.10072 factor:1 | -1 (0.31952) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.37337 HOMO: -6.42189 LUMO: 2.19596 factor:1 | -1 (0.00103) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.13470 HOMO: -6.40556 LUMO: 2.02181 factor:1 | -1 (0.23971) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.05238 HOMO: -6.41372 LUMO: 2.26671 factor:1 | -1 (0.32202) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.93488 HOMO: -6.60692 LUMO: 2.09800 factor:1 | -1 (0.43952) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.31906 HOMO: -6.75931 LUMO: 1.76602 factor:1 | -1 (0.05535) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92688 HOMO: -6.39195 LUMO: 1.84221 factor:1 | -1 (0.44752) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.84351 HOMO: -6.74570 LUMO: 2.04085 factor:1 | -1 (0.53089) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.73877 HOMO: -6.77019 LUMO: 2.16875 factor:1 | -1 (0.63563) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.13905 HOMO: -6.15522 LUMO: 1.81772 factor:1 | -1 (0.23535) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19685 HOMO: -6.48175 LUMO: 2.02453 factor:1 | -1 (0.17755) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16787 HOMO: -6.57427 LUMO: 1.77962 factor:1 | -1 (0.20653) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.46178 HOMO: -6.57699 LUMO: 2.42998 factor:1 | 1 (-0.08738) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25873 HOMO: -6.35386 LUMO: 2.25310 factor:1 | -1 (0.11568) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17415 HOMO: -6.80013 LUMO: 2.11160 factor:1 | -1 (0.20025) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14071 HOMO: -6.24229 LUMO: 2.05718 factor:1 | -1 (0.23369) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.95148 HOMO: -6.42733 LUMO: 1.76874 factor:1 | -1 (0.42292) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01083 HOMO: -6.56883 LUMO: 2.36195 factor:1 | -1 (0.36357) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.00787 HOMO: -6.72665 LUMO: 2.28848 factor:1 | -1 (0.36654) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19168 HOMO: -6.39195 LUMO: 1.79051 factor:1 | -1 (0.18272) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.23791 HOMO: -6.70761 LUMO: 0.15510 factor:1 | -1 (0.13649) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04798 HOMO: -6.44366 LUMO: -0.16871 factor:1 | -1 (0.32643) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17467 HOMO: -6.68584 LUMO: 1.69527 factor:1 | -1 (0.19973) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.24763 HOMO: -6.26950 LUMO: 1.61636 factor:1 | -1 (0.12678) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02925 HOMO: -6.47631 LUMO: 1.98915 factor:1 | -1 (0.34515) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.13630 HOMO: -6.58243 LUMO: 1.97283 factor:1 | -1 (0.23810) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.90547 HOMO: -6.51713 LUMO: 1.97283 factor:1 | -1 (0.46893) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.12403 HOMO: -6.65046 LUMO: 1.69255 factor:1 | -1 (0.25037) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92683 HOMO: -6.26406 LUMO: 2.21773 factor:1 | -1 (0.44757) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.01540 HOMO: -6.88992 LUMO: 2.28304 factor:1 | -1 (0.35900) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.85159 HOMO: -6.67767 LUMO: 2.34834 factor:1 | -1 (0.52281) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04866 HOMO: -6.52801 LUMO: 2.10344 factor:1 | -1 (0.32575) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.86686 HOMO: -6.52801 LUMO: 2.24222 factor:1 | -1 (0.50755) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.81072 HOMO: -6.17154 LUMO: 1.89663 factor:1 | -1 (0.56368) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.66941 HOMO: -6.42733 LUMO: 2.15514 factor:1 | -1 (0.70499) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.12479 HOMO: -6.36474 LUMO: 2.01364 factor:1 | -1 (0.24961) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.92645 HOMO: -6.82189 LUMO: 1.86942 factor:1 | -1 (0.44795) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.71687 HOMO: -6.60148 LUMO: 2.00548 factor:1 | -1 (0.65754) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02000 HOMO: -6.67767 LUMO: 2.15786 factor:1 | -1 (0.35440) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.82326 HOMO: -6.79196 LUMO: 2.06534 factor:1 | -1 (0.55114) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.18474 HOMO: -6.70216 LUMO: 1.83405 factor:1 | -1 (0.18966) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02425 HOMO: -6.58788 LUMO: 1.79051 factor:1 | -1 (0.35016) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.18354 HOMO: -6.34842 LUMO: 1.80139 factor:1 | -1 (0.19086) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.11456 HOMO: -6.48175 LUMO: 1.95922 factor:1 | -1 (0.25984) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.73349 HOMO: -6.71033 LUMO: 2.02997 factor:1 | -1 (0.64091) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.14166 HOMO: -6.89264 LUMO: 2.42726 factor:1 | -1 (0.23274) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09179 HOMO: -6.74570 LUMO: 2.20684 factor:1 | -1 (0.28262) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.30305 HOMO: -6.30216 LUMO: 2.15242 factor:1 | -1 (0.07135) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.37024 HOMO: -6.94979 LUMO: 2.43814 factor:1 | -1 (0.00416) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.25579 HOMO: -6.97972 LUMO: 2.11432 factor:1 | -1 (0.11861) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.10471 HOMO: -6.17154 LUMO: 1.98099 factor:1 | -1 (0.26969) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.88337 HOMO: -6.74026 LUMO: 2.21501 factor:1 | -1 (0.49103) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.08047 HOMO: -6.72393 LUMO: 2.19596 factor:1 | -1 (0.29394) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.08572 HOMO: -6.11440 LUMO: 2.10072 factor:1 | -1 (0.28869) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09391 HOMO: -6.34297 LUMO: 1.92657 factor:1 | -1 (0.28049) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.88343 HOMO: -6.24773 LUMO: 2.00276 factor:1 | -1 (0.49098) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.24303 HOMO: -6.75114 LUMO: 1.98643 factor:1 | -1 (0.13138) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.03940 HOMO: -6.69128 LUMO: 2.08711 factor:1 | -1 (0.33500) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.32017 HOMO: -6.65318 LUMO: 2.15514 factor:1 | -1 (0.05423) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17837 HOMO: -6.67495 LUMO: 1.72248 factor:1 | -1 (0.19603) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04196 HOMO: -6.58243 LUMO: 1.83405 factor:1 | -1 (0.33244) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.90405 HOMO: -6.61237 LUMO: 1.69799 factor:1 | -1 (0.47035) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.17426 HOMO: -6.57427 LUMO: 2.29936 factor:1 | -1 (0.20014) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02716 HOMO: -6.40012 LUMO: 2.35378 factor:1 | -1 (0.34724) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.93080 HOMO: -6.90081 LUMO: 2.26671 factor:1 | -1 (0.44360) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.19622 HOMO: -6.44910 LUMO: 2.25855 factor:1 | -1 (0.17818) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.97954 HOMO: -6.61509 LUMO: 2.26943 factor:1 | -1 (0.39486) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87916 HOMO: -6.78924 LUMO: 2.09256 factor:1 | -1 (0.49525) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.78416 HOMO: -6.47087 LUMO: 1.97555 factor:1 | -1 (0.59024) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.08776 HOMO: -6.75931 LUMO: 1.98643 factor:1 | -1 (0.28664) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04112 HOMO: -6.17971 LUMO: 2.09800 factor:1 | -1 (0.33329) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.12063 HOMO: -6.83006 LUMO: 1.91840 factor:1 | -1 (0.25377) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.24077 HOMO: -6.72938 LUMO: 2.17419 factor:1 | -1 (0.13364) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.16909 HOMO: -6.78924 LUMO: 2.42726 factor:1 | -1 (0.20531) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.18188 HOMO: -6.41372 LUMO: 1.93745 factor:1 | -1 (0.19252) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.18934 HOMO: -6.85455 LUMO: 2.14970 factor:1 | -1 (0.18506) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.03078 HOMO: -6.38651 LUMO: 2.18507 factor:1 | -1 (0.34363) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.04847 HOMO: -6.81373 LUMO: 2.00548 factor:1 | -1 (0.32594) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.89839 HOMO: -6.64774 LUMO: 2.41365 factor:1 | -1 (0.47601) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.82857 HOMO: -6.70489 LUMO: 2.31569 factor:1 | -1 (0.54583) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.09902 HOMO: -6.49264 LUMO: 1.78779 factor:1 | -1 (0.27538) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.99665 HOMO: -6.81101 LUMO: 1.86670 factor:1 | -1 (0.37775) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.78813 HOMO: -6.72121 LUMO: 1.48846 factor:1 | -1 (0.58627) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02357 HOMO: -6.35930 LUMO: 1.78507 factor:1 | -1 (0.35084) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.80661 HOMO: -6.38651 LUMO: 2.04358 factor:1 | -1 (0.56779) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.93714 HOMO: -6.42189 LUMO: 1.99187 factor:1 | -1 (0.43726) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.02183 HOMO: -6.69400 LUMO: 1.61091 factor:1 | -1 (0.35258) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.83499 HOMO: -6.81101 LUMO: 2.17419 factor:1 | -1 (0.53941) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.96229 HOMO: -6.90897 LUMO: 2.28576 factor:1 | -1 (0.41212) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.87624 HOMO: -6.75387 LUMO: 2.31297 factor:1 | -1 (0.49816) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11609.68196 HOMO: -7.05863 LUMO: 2.18780 factor:1 | -1 (0.69245) | -1 | -1 |
| G: -5346.00871 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11610.06613 HOMO: -6.56611 LUMO: 1.99187 factor:1 | -1 (0.30828) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01612 HOMO: -6.59060 LUMO: 1.86398 factor:1 | 1 (-3.27005) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.91712 HOMO: -6.59060 LUMO: 1.59459 factor:1 | 1 (-3.17105) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.97000 HOMO: -6.57699 LUMO: 1.48030 factor:1 | 1 (-3.22392) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.02096 HOMO: -6.99605 LUMO: 2.30208 factor:1 | 1 (-3.27489) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.04543 HOMO: -6.42189 LUMO: 2.20412 factor:1 | 1 (-3.29935) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.97174 HOMO: -7.15115 LUMO: 1.83405 factor:1 | 1 (-3.22566) | 1 | 1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.07544 HOMO: -7.08040 LUMO: 2.21773 factor:1 | 1 (-3.32937) | 1 | 1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.18592 HOMO: -6.72121 LUMO: 1.89663 factor:1 | 1 (-3.43985) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.08303 HOMO: -6.25590 LUMO: 1.85037 factor:1 | 1 (-3.33696) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.91078 HOMO: -6.70489 LUMO: 1.98915 factor:1 | 1 (-3.16471) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.90485 HOMO: -6.53617 LUMO: 2.08439 factor:1 | 1 (-3.15878) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.95266 HOMO: -6.69944 LUMO: 1.98915 factor:1 | 1 (-3.20659) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68667 HOMO: -6.79468 LUMO: 1.96466 factor:1 | 1 (-2.94060) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.85895 HOMO: -6.79468 LUMO: 1.99459 factor:1 | 1 (-3.11287) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.41425 HOMO: -6.58788 LUMO: 1.98371 factor:1 | 1 (-3.66818) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.82820 HOMO: -6.58788 LUMO: 2.16603 factor:1 | 1 (-3.08212) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.91601 HOMO: -6.56883 LUMO: 1.64085 factor:1 | 1 (-3.16994) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.59581 HOMO: -7.19197 LUMO: 2.66127 factor:1 | 1 (-2.84974) | 1 | 1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.70166 HOMO: -6.48175 LUMO: 2.40004 factor:1 | 1 (-2.95559) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.80920 HOMO: -6.18515 LUMO: 2.27759 factor:1 | 1 (-3.06313) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52419 HOMO: -6.64774 LUMO: 2.13337 factor:1 | 1 (-2.77812) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.06336 HOMO: -6.39740 LUMO: 1.95106 factor:1 | 1 (-3.31729) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.13672 HOMO: -6.59332 LUMO: 1.81772 factor:1 | 1 (-3.39065) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.93560 HOMO: -6.68312 LUMO: 2.41909 factor:1 | 1 (-3.18953) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.17743 HOMO: -5.87494 LUMO: 2.18235 factor:1 | 1 (-3.43136) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.23737 HOMO: -6.30488 LUMO: 2.04902 factor:1 | 1 (-3.49130) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.03016 HOMO: -6.65046 LUMO: 2.05446 factor:1 | 1 (-3.28409) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.16227 HOMO: -6.55794 LUMO: 2.06807 factor:1 | 1 (-3.41620) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.96151 HOMO: -6.68040 LUMO: 1.99187 factor:1 | 1 (-3.21543) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.08521 HOMO: -6.60965 LUMO: 2.18780 factor:1 | 1 (-3.33914) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.80645 HOMO: -6.88176 LUMO: 2.10344 factor:1 | 1 (-3.06038) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.87835 HOMO: -6.63414 LUMO: 1.70615 factor:1 | 1 (-3.13228) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.88708 HOMO: -7.15115 LUMO: 2.07351 factor:1 | 1 (-3.14101) | 1 | 1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.67083 HOMO: -6.85727 LUMO: 2.27759 factor:1 | 1 (-2.92476) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.75225 HOMO: -6.91713 LUMO: 2.28848 factor:1 | 1 (-3.00618) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.19084 HOMO: -7.10217 LUMO: 2.14698 factor:1 | 1 (-3.44477) | 1 | 1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.24529 HOMO: -6.78108 LUMO: 2.45447 factor:1 | 1 (-3.49922) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.06251 HOMO: -6.78380 LUMO: 2.43542 factor:1 | 1 (-3.31644) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.93522 HOMO: -6.60965 LUMO: 2.33474 factor:1 | 1 (-3.18915) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72267 HOMO: -6.72665 LUMO: 2.25855 factor:1 | 1 (-2.97660) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.89794 HOMO: -6.27495 LUMO: 2.04358 factor:1 | 1 (-3.15187) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.77538 HOMO: -6.17426 LUMO: 1.45853 factor:1 | 1 (-3.02931) | -1 | -1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.03726 HOMO: -7.21374 LUMO: 2.33474 factor:1 | 1 (-3.29119) | 1 | 1 |
| G: -5245.38038 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.88768 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-3.14161) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.05435 HOMO: -6.80829 LUMO: 0.17960 factor:1 | 1 (-3.30828) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.10826 HOMO: -7.19469 LUMO: 1.60819 factor:1 | 1 (-3.36218) | 1 | 1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.89979 HOMO: -6.78652 LUMO: 0.53334 factor:1 | 1 (-3.15372) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.75704 HOMO: -6.70489 LUMO: 0.74559 factor:1 | 1 (-3.01097) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60637 HOMO: -6.72393 LUMO: 0.88981 factor:1 | 1 (-2.86030) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.95576 HOMO: -4.54430 LUMO: -0.90614 factor:1 | 1 (-3.20969) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.97236 HOMO: -6.83006 LUMO: 0.47348 factor:1 | 1 (-3.22629) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.92537 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-3.17930) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65957 HOMO: -6.62053 LUMO: 0.74559 factor:1 | 1 (-2.91350) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.95835 HOMO: -6.79196 LUMO: 1.80139 factor:1 | 1 (-3.21228) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.84371 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-3.09764) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.70349 HOMO: -6.74026 LUMO: 0.95784 factor:1 | 1 (-2.95742) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.97595 HOMO: -7.34707 LUMO: 0.40001 factor:1 | 1 (-3.22988) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.96929 HOMO: -6.19875 LUMO: -0.88709 factor:1 | 1 (-3.22322) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.96194 HOMO: -6.48719 LUMO: -0.14694 factor:1 | 1 (-3.21587) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.66855 HOMO: -6.73482 LUMO: -0.01633 factor:1 | 1 (-2.92248) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.08709 HOMO: -7.05591 LUMO: -0.20136 factor:1 | 1 (-3.34101) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.04352 HOMO: -6.38651 LUMO: -2.07895 factor:1 | 1 (-3.29745) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.78689 HOMO: -6.85455 LUMO: -1.03403 factor:1 | 1 (-3.04082) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.98001 HOMO: -6.72121 LUMO: -0.99322 factor:1 | 1 (-3.23394) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.89103 HOMO: -6.53890 LUMO: -0.10885 factor:1 | 1 (-3.14496) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72213 HOMO: -6.68312 LUMO: 0.21225 factor:1 | 1 (-2.97605) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.85097 HOMO: -6.68040 LUMO: 0.21225 factor:1 | 1 (-3.10490) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.78890 HOMO: -6.76475 LUMO: -0.64491 factor:1 | 1 (-3.04283) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.59976 HOMO: -6.48175 LUMO: 0.41633 factor:1 | 1 (-2.85369) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.77916 HOMO: -6.42733 LUMO: 0.16599 factor:1 | 1 (-3.03309) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65682 HOMO: -6.66679 LUMO: 0.77825 factor:1 | 1 (-2.91075) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.61837 HOMO: -6.75931 LUMO: -0.73471 factor:1 | 1 (-2.87230) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.80145 HOMO: -6.53617 LUMO: 0.38096 factor:1 | 1 (-3.05538) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60427 HOMO: -6.34297 LUMO: 0.35375 factor:1 | 1 (-2.85820) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60183 HOMO: -7.11850 LUMO: -0.03265 factor:1 | 1 (-2.85575) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50438 HOMO: -5.21914 LUMO: 1.29798 factor:1 | 1 (-2.75831) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68906 HOMO: -7.09129 LUMO: -0.66668 factor:1 | 1 (-2.94299) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90373 HOMO: -6.96884 LUMO: -0.31021 factor:1 | 1 (-1.15765) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70269 HOMO: -6.51713 LUMO: -0.59865 factor:1 | 1 (-0.95662) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.94452 HOMO: -6.69400 LUMO: -0.07075 factor:1 | 1 (-1.19844) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71395 HOMO: -5.28173 LUMO: 1.17281 factor:1 | 1 (-0.96788) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64203 HOMO: -6.54434 LUMO: 0.32109 factor:1 | 1 (-0.89596) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85377 HOMO: -6.79740 LUMO: -0.24762 factor:1 | 1 (-1.10769) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21268 HOMO: -6.91986 LUMO: -0.14694 factor:1 | 1 (-1.46661) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.98487 HOMO: -6.75114 LUMO: 0.18504 factor:1 | 1 (-1.23880) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11597 HOMO: -6.74842 LUMO: 0.69389 factor:1 | 1 (-1.36990) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30354 HOMO: -7.01782 LUMO: 0.56600 factor:1 | 1 (-1.55747) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14215 HOMO: -6.47359 LUMO: -0.56600 factor:1 | 1 (-1.39608) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26479 HOMO: -6.63686 LUMO: -0.55783 factor:1 | 1 (-1.51872) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17143 HOMO: -4.13885 LUMO: -2.05446 factor:1 | 1 (-1.42536) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76195 HOMO: -6.34570 LUMO: 0.19864 factor:1 | 1 (-1.01588) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.18491 HOMO: -6.47903 LUMO: 0.24762 factor:1 | 1 (-0.43884) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10687 HOMO: -6.15249 LUMO: 0.32109 factor:1 | 1 (-0.36080) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.98137 HOMO: -6.84366 LUMO: 0.29116 factor:1 | 1 (-0.23530) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.15664 HOMO: -6.34297 LUMO: 0.19864 factor:1 | 1 (-0.41057) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.04485 HOMO: -6.51168 LUMO: 0.30749 factor:1 | 1 (-0.29878) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.52705 HOMO: -6.79468 LUMO: -0.16599 factor:1 | -1 (0.21902) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.11998 HOMO: -7.24095 LUMO: 0.15238 factor:1 | 1 (-0.37391) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.03892 HOMO: -7.06952 LUMO: -0.34558 factor:1 | 1 (-0.29285) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37457 HOMO: -6.88176 LUMO: 0.02177 factor:1 | 1 (-0.62850) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.79277 HOMO: -6.37291 LUMO: -0.69117 factor:1 | 1 (-0.04669) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38722 HOMO: -6.83278 LUMO: -0.59049 factor:1 | 1 (-1.64115) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.24130 HOMO: -6.57155 LUMO: -0.33470 factor:1 | -1 (0.50477) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.23052 HOMO: -6.89537 LUMO: -0.58504 factor:1 | -1 (0.51555) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.96964 HOMO: -6.57155 LUMO: -0.34831 factor:1 | 1 (-0.22357) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.78028 HOMO: -6.64774 LUMO: -0.95784 factor:1 | 1 (-0.03420) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.20260 HOMO: -6.91713 LUMO: -0.69933 factor:1 | 1 (-0.45653) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.05114 HOMO: -6.80557 LUMO: -0.65035 factor:1 | 1 (-0.30507) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.01862 HOMO: -7.26544 LUMO: -0.79729 factor:1 | 1 (-0.27255) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39062 HOMO: -6.69128 LUMO: -0.16871 factor:1 | 1 (-1.64455) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48670 HOMO: -6.88448 LUMO: 0.13061 factor:1 | 1 (-1.74063) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33558 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-0.58951) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21332 HOMO: -6.56067 LUMO: 0.17687 factor:1 | 1 (-0.46725) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.07669 HOMO: -6.70216 LUMO: 0.25034 factor:1 | 1 (-0.33062) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55028 HOMO: -6.51713 LUMO: -0.78369 factor:1 | 1 (-0.80421) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65953 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-0.91346) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.95905 HOMO: -6.22052 LUMO: -0.83811 factor:1 | 1 (-1.21297) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63357 HOMO: -6.51168 LUMO: -0.76464 factor:1 | 1 (-0.88750) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75553 HOMO: -7.14571 LUMO: -0.80274 factor:1 | 1 (-1.00946) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.68193 HOMO: -6.66679 LUMO: -0.88709 factor:1 | 1 (-0.93585) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09793 HOMO: -6.76203 LUMO: -1.43948 factor:1 | 1 (-1.35186) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65732 HOMO: -6.57427 LUMO: -1.62996 factor:1 | 1 (-1.91125) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50572 HOMO: -5.05043 LUMO: 1.24900 factor:1 | 1 (-1.75965) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59655 HOMO: -6.53345 LUMO: 0.23130 factor:1 | 1 (-1.85048) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68894 HOMO: -7.18381 LUMO: -0.22585 factor:1 | 1 (-1.94287) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98432 HOMO: -7.00965 LUMO: -1.79595 factor:1 | 1 (-2.23825) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44801 HOMO: -6.08174 LUMO: -0.82995 factor:1 | 1 (-1.70194) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39987 HOMO: -6.42189 LUMO: -0.84355 factor:1 | 1 (-1.65380) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58583 HOMO: -6.53890 LUMO: 0.60409 factor:1 | 1 (-1.83976) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73171 HOMO: -6.62869 LUMO: 0.43810 factor:1 | 1 (-1.98564) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73740 HOMO: -6.68312 LUMO: 0.64491 factor:1 | 1 (-1.99133) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59851 HOMO: -6.42189 LUMO: 1.51295 factor:1 | 1 (-1.85244) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52439 HOMO: -6.17971 LUMO: 1.67622 factor:1 | 1 (-1.77832) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71299 HOMO: -6.79196 LUMO: 1.36873 factor:1 | 1 (-1.96692) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73014 HOMO: -7.38517 LUMO: 0.56328 factor:1 | 1 (-1.98406) | 1 | 1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85417 HOMO: -7.56204 LUMO: 0.71566 factor:1 | 1 (-1.10810) | 1 | 1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01420 HOMO: -6.45726 LUMO: -1.91840 factor:1 | 1 (-1.26813) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84903 HOMO: -6.13073 LUMO: -0.97417 factor:1 | 1 (-1.10296) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.95545 HOMO: -6.50352 LUMO: -0.69661 factor:1 | 1 (-1.20938) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83762 HOMO: -6.76747 LUMO: -1.71976 factor:1 | 1 (-2.09155) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95629 HOMO: -6.48447 LUMO: -0.89525 factor:1 | 1 (-2.21022) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58156 HOMO: -7.11850 LUMO: -0.71566 factor:1 | 1 (-1.83549) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62439 HOMO: -6.80285 LUMO: -0.49253 factor:1 | 1 (-1.87832) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84875 HOMO: -6.80557 LUMO: -0.88165 factor:1 | 1 (-2.10268) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.92805 HOMO: -6.94162 LUMO: -0.08980 factor:1 | 1 (-1.18198) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.87023 HOMO: -6.97972 LUMO: -0.29388 factor:1 | 1 (-1.12416) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03932 HOMO: -6.75114 LUMO: 0.04626 factor:1 | 1 (-1.29325) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72897 HOMO: -7.15932 LUMO: 0.68845 factor:1 | 1 (-0.98290) | 1 | 1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76944 HOMO: -7.36612 LUMO: 0.63675 factor:1 | 1 (-1.02337) | 1 | 1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77874 HOMO: -7.02598 LUMO: -0.66124 factor:1 | 1 (-1.03267) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42619 HOMO: -6.89264 LUMO: -0.54967 factor:1 | 1 (-0.68012) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.30897 HOMO: -6.97700 LUMO: 0.27756 factor:1 | 1 (-0.56289) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.95348 HOMO: -6.60965 LUMO: 0.08163 factor:1 | 1 (-0.20741) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.03849 HOMO: -6.70761 LUMO: 0.40001 factor:1 | 1 (-0.29241) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.13155 HOMO: -6.69128 LUMO: 0.23674 factor:1 | 1 (-0.38548) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.99470 HOMO: -6.69128 LUMO: -0.69933 factor:1 | 1 (-0.24863) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.26456 HOMO: -6.18515 LUMO: -0.85988 factor:1 | 1 (-0.51849) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.14328 HOMO: -6.86815 LUMO: -1.90208 factor:1 | 1 (-0.39720) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28286 HOMO: -6.37563 LUMO: -1.74697 factor:1 | 1 (-1.53679) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01102 HOMO: -6.75659 LUMO: 0.36463 factor:1 | 1 (-1.26495) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14672 HOMO: -6.91441 LUMO: -0.88981 factor:1 | 1 (-1.40065) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33696 HOMO: -6.71305 LUMO: -0.29933 factor:1 | 1 (-1.59089) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03573 HOMO: -6.91441 LUMO: -1.04492 factor:1 | 1 (-1.28966) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12882 HOMO: -6.05453 LUMO: -0.83539 factor:1 | 1 (-1.38275) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33221 HOMO: -7.35252 LUMO: -0.45715 factor:1 | 1 (-0.58613) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27093 HOMO: -6.41644 LUMO: -0.97417 factor:1 | 1 (-0.52485) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27405 HOMO: -6.78924 LUMO: 0.36735 factor:1 | 1 (-0.52798) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.05759 HOMO: -6.74298 LUMO: 0.51974 factor:1 | 1 (-0.31152) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.87992 HOMO: -6.48992 LUMO: 1.44765 factor:1 | 1 (-0.13385) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.84039 HOMO: -6.12528 LUMO: 1.57826 factor:1 | 1 (-0.09431) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09557 HOMO: -6.62325 LUMO: 1.57826 factor:1 | 1 (-1.34949) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34425 HOMO: -6.19875 LUMO: 1.29798 factor:1 | 1 (-1.59818) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11913 HOMO: -6.74570 LUMO: 1.52112 factor:1 | 1 (-1.37306) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11573 HOMO: -6.84094 LUMO: 1.48574 factor:1 | 1 (-1.36966) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71860 HOMO: -6.85183 LUMO: 0.33470 factor:1 | 1 (-1.97253) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41457 HOMO: -6.51168 LUMO: 0.48164 factor:1 | 1 (-1.66849) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45359 HOMO: -6.25046 LUMO: 0.75648 factor:1 | 1 (-1.70751) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49400 HOMO: -6.65591 LUMO: 0.32109 factor:1 | 1 (-0.74793) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10869 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-0.36262) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.98983 HOMO: -6.75114 LUMO: 0.73471 factor:1 | 1 (-0.24376) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32700 HOMO: -6.50624 LUMO: 0.59321 factor:1 | 1 (-1.58093) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02520 HOMO: -6.39740 LUMO: 0.83267 factor:1 | 1 (-1.27913) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41693 HOMO: -6.44094 LUMO: 0.65579 factor:1 | 1 (-1.67086) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22196 HOMO: -6.52257 LUMO: 0.05714 factor:1 | 1 (-1.47589) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14452 HOMO: -7.10217 LUMO: 0.49797 factor:1 | 1 (-1.39845) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09815 HOMO: -6.83006 LUMO: 0.55783 factor:1 | 1 (-1.35208) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.93102 HOMO: -6.99333 LUMO: -0.79457 factor:1 | 1 (-1.18495) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88196 HOMO: -6.64230 LUMO: 0.32382 factor:1 | 1 (-1.13588) | -1 | -1 |
| G: -5245.38038 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40368 HOMO: -6.90897 LUMO: 0.30749 factor:1 | 1 (-1.65761) | -1 | -1 |
| G: -5245.38038 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62976 HOMO: -7.09129 LUMO: 1.33336 factor:1 | 1 (-0.88369) | 1 | 1 |
| G: -5245.38038 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.77380 HOMO: -6.66951 LUMO: 1.34424 factor:1 | 1 (-3.02773) | -1 | -1 |
| G: -5245.38038 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.90311 HOMO: -7.02870 LUMO: 1.48574 factor:1 | 1 (-3.15704) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.86714 HOMO: -7.26544 LUMO: 0.32926 factor:1 | 1 (-3.12106) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72607 HOMO: -6.56067 LUMO: -0.45987 factor:1 | 1 (-2.98000) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.97869 HOMO: -6.54434 LUMO: -0.28300 factor:1 | 1 (-1.23262) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23745 HOMO: -7.19469 LUMO: 0.54695 factor:1 | 1 (-1.49137) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49680 HOMO: -6.47359 LUMO: -0.22041 factor:1 | 1 (-1.75073) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83981 HOMO: -6.80013 LUMO: 2.08167 factor:1 | 1 (-1.09373) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.93431 HOMO: -6.23957 LUMO: 1.67894 factor:1 | 1 (-1.18824) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13089 HOMO: -6.75114 LUMO: -0.62858 factor:1 | 1 (-1.38481) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88890 HOMO: -6.79468 LUMO: -0.64491 factor:1 | 1 (-1.14282) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83812 HOMO: -6.84911 LUMO: -0.69661 factor:1 | 1 (-1.09205) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44752 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-1.70145) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85079 HOMO: -6.92802 LUMO: -0.71022 factor:1 | 1 (-2.10472) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15997 HOMO: -6.72665 LUMO: -0.46804 factor:1 | 1 (-2.41389) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.23039 HOMO: -6.63686 LUMO: -0.23674 factor:1 | 1 (-2.48432) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.17349 HOMO: -7.21102 LUMO: 0.54423 factor:1 | 1 (-2.42742) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94483 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-2.19876) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.21387 HOMO: -6.70761 LUMO: -0.31837 factor:1 | 1 (-2.46780) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00347 HOMO: -6.57155 LUMO: 1.76874 factor:1 | 1 (-2.25740) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90652 HOMO: -6.84366 LUMO: 2.04358 factor:1 | 1 (-2.16045) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91985 HOMO: -6.60420 LUMO: 1.80139 factor:1 | 1 (-2.17378) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80448 HOMO: -7.03686 LUMO: 2.21229 factor:1 | 1 (-2.05841) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80339 HOMO: -6.77564 LUMO: 1.97555 factor:1 | 1 (-2.05732) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60439 HOMO: -6.40012 LUMO: 2.17691 factor:1 | 1 (-1.85832) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.01259 HOMO: -6.80013 LUMO: 2.25582 factor:1 | 1 (-2.26652) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03161 HOMO: -6.74298 LUMO: 2.31569 factor:1 | 1 (-2.28554) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.96162 HOMO: -6.68856 LUMO: 1.85854 factor:1 | 1 (-2.21555) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81800 HOMO: -6.17971 LUMO: 1.52928 factor:1 | 1 (-2.07193) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98383 HOMO: -6.54162 LUMO: 1.91840 factor:1 | 1 (-2.23776) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98502 HOMO: -6.80013 LUMO: -0.55511 factor:1 | 1 (-2.23895) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.96124 HOMO: -7.46953 LUMO: 0.28572 factor:1 | 1 (-2.21517) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94173 HOMO: -6.61781 LUMO: -0.54967 factor:1 | 1 (-2.19566) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.18500 HOMO: -6.56339 LUMO: -0.47892 factor:1 | 1 (-2.43893) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88600 HOMO: -6.65591 LUMO: -0.25307 factor:1 | 1 (-2.13993) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.29540 HOMO: -6.62869 LUMO: -0.23402 factor:1 | 1 (-2.54933) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97085 HOMO: -6.58243 LUMO: -0.19048 factor:1 | 1 (-2.22478) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.23869 HOMO: -7.27632 LUMO: 0.52790 factor:1 | 1 (-2.49262) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96166 HOMO: -7.21102 LUMO: 0.57688 factor:1 | 1 (-1.21559) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.68582 HOMO: -6.72393 LUMO: -0.53879 factor:1 | 1 (-0.93975) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17829 HOMO: -7.42054 LUMO: -0.99322 factor:1 | 1 (-1.43222) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14743 HOMO: -6.88992 LUMO: -0.71838 factor:1 | 1 (-1.40136) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01660 HOMO: -6.88176 LUMO: -0.61226 factor:1 | 1 (-1.27053) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11924 HOMO: -7.36340 LUMO: -1.04492 factor:1 | 1 (-1.37317) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57484 HOMO: -6.65863 LUMO: -0.41906 factor:1 | 1 (-1.82877) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38213 HOMO: -7.15115 LUMO: -0.66396 factor:1 | 1 (-1.63606) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45073 HOMO: -7.10489 LUMO: -0.64491 factor:1 | 1 (-1.70466) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47525 HOMO: -7.20285 LUMO: 0.47892 factor:1 | 1 (-1.72917) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57408 HOMO: -6.55794 LUMO: -0.28844 factor:1 | 1 (-1.82801) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39685 HOMO: -7.19197 LUMO: -0.69661 factor:1 | 1 (-1.65078) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72635 HOMO: -6.56883 LUMO: -0.32926 factor:1 | 1 (-1.98028) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00549 HOMO: -6.70761 LUMO: 1.95650 factor:1 | 1 (-2.25942) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77030 HOMO: -6.60420 LUMO: 1.80684 factor:1 | 1 (-2.02423) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73231 HOMO: -6.84094 LUMO: 1.64085 factor:1 | 1 (-1.98624) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94336 HOMO: -6.69128 LUMO: 1.90208 factor:1 | 1 (-2.19729) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03428 HOMO: -6.75387 LUMO: 1.70343 factor:1 | 1 (-2.28821) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95885 HOMO: -7.07496 LUMO: 2.10072 factor:1 | 1 (-2.21278) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92187 HOMO: -6.99877 LUMO: 2.24494 factor:1 | 1 (-2.17580) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08694 HOMO: -6.63414 LUMO: 2.17691 factor:1 | 1 (-1.34087) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.98833 HOMO: -6.44638 LUMO: 1.78235 factor:1 | 1 (-1.24225) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12738 HOMO: -6.87632 LUMO: 1.84221 factor:1 | 1 (-1.38130) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19211 HOMO: -6.85183 LUMO: 1.68711 factor:1 | 1 (-1.44604) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10833 HOMO: -6.96339 LUMO: 2.26671 factor:1 | 1 (-1.36226) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04128 HOMO: -6.63141 LUMO: 1.96738 factor:1 | 1 (-1.29521) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.91235 HOMO: -6.37019 LUMO: 2.23133 factor:1 | 1 (-1.16628) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88792 HOMO: -7.11034 LUMO: 2.32385 factor:1 | 1 (-1.14184) | 1 | 1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88337 HOMO: -6.91986 LUMO: 1.65445 factor:1 | 1 (-1.13730) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32357 HOMO: -7.12938 LUMO: 2.28304 factor:1 | 1 (-1.57750) | 1 | 1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02180 HOMO: -6.54978 LUMO: 1.92112 factor:1 | 1 (-1.27572) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90326 HOMO: -6.83006 LUMO: 2.48712 factor:1 | 1 (-1.15719) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06109 HOMO: -6.97972 LUMO: 1.96738 factor:1 | 1 (-1.31502) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96179 HOMO: -6.69944 LUMO: 2.06262 factor:1 | 1 (-1.21572) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04996 HOMO: -6.76747 LUMO: 2.10888 factor:1 | 1 (-1.30389) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38738 HOMO: -6.91169 LUMO: 2.06534 factor:1 | 1 (-1.64131) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38521 HOMO: -7.03414 LUMO: 1.93473 factor:1 | 1 (-0.63914) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17035 HOMO: -7.03142 LUMO: 2.52250 factor:1 | 1 (-0.42428) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.08298 HOMO: -6.34025 LUMO: 2.61229 factor:1 | 1 (-0.33690) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.09351 HOMO: -6.98788 LUMO: 2.28304 factor:1 | 1 (-0.34743) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.93916 HOMO: -6.97700 LUMO: 2.53882 factor:1 | 1 (-0.19309) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42097 HOMO: -6.58788 LUMO: 1.94289 factor:1 | 1 (-0.67490) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.30007 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-0.55400) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15900 HOMO: -6.55250 LUMO: 1.82861 factor:1 | 1 (-1.41292) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04874 HOMO: -6.45998 LUMO: 1.75786 factor:1 | 1 (-1.30266) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85687 HOMO: -6.78924 LUMO: 2.33746 factor:1 | 1 (-1.11080) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30145 HOMO: -6.85727 LUMO: 1.76058 factor:1 | 1 (-1.55538) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41258 HOMO: -6.70489 LUMO: 1.84493 factor:1 | 1 (-1.66651) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19829 HOMO: -6.71305 LUMO: 1.53472 factor:1 | 1 (-1.45222) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89562 HOMO: -6.76747 LUMO: 1.48846 factor:1 | 1 (-1.14955) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17535 HOMO: -6.69128 LUMO: 1.95922 factor:1 | 1 (-1.42928) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89409 HOMO: -6.67495 LUMO: 2.05446 factor:1 | 1 (-1.14802) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73638 HOMO: -6.63686 LUMO: 2.25310 factor:1 | 1 (-0.99030) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.61692 HOMO: -6.63958 LUMO: 2.14154 factor:1 | 1 (-0.87085) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20678 HOMO: -6.62597 LUMO: 2.01908 factor:1 | 1 (-1.46071) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59620 HOMO: -7.07768 LUMO: 2.14154 factor:1 | 1 (-1.85013) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34752 HOMO: -6.19603 LUMO: 2.01092 factor:1 | 1 (-1.60144) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60959 HOMO: -6.65046 LUMO: 2.15786 factor:1 | 1 (-1.86352) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04680 HOMO: -6.92258 LUMO: 2.31841 factor:1 | 1 (-1.30073) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12400 HOMO: -6.90081 LUMO: 2.19324 factor:1 | 1 (-1.37793) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27086 HOMO: -6.85455 LUMO: 1.95650 factor:1 | 1 (-1.52479) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.97946 HOMO: -6.57699 LUMO: 1.76058 factor:1 | 1 (-1.23338) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11004 HOMO: -6.90625 LUMO: 1.97555 factor:1 | 1 (-1.36397) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12446 HOMO: -6.97428 LUMO: 1.92929 factor:1 | 1 (-1.37839) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88551 HOMO: -6.61781 LUMO: -0.41906 factor:1 | 1 (-2.13944) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.10900 HOMO: -6.62869 LUMO: -0.81906 factor:1 | 1 (-2.36293) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94960 HOMO: -7.01237 LUMO: 2.00548 factor:1 | 1 (-2.20352) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12639 HOMO: -6.85727 LUMO: 2.17691 factor:1 | 1 (-2.38032) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78589 HOMO: -6.71849 LUMO: 1.58914 factor:1 | 1 (-2.03982) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95221 HOMO: -7.52395 LUMO: 0.27211 factor:1 | 1 (-2.20614) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62524 HOMO: -6.96611 LUMO: -0.72654 factor:1 | 1 (-1.87916) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67443 HOMO: -6.89537 LUMO: -0.68028 factor:1 | 1 (-1.92836) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64668 HOMO: -6.84911 LUMO: -0.58504 factor:1 | 1 (-1.90061) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84782 HOMO: -6.79196 LUMO: -0.55783 factor:1 | 1 (-2.10175) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79196 HOMO: -6.67767 LUMO: 1.79323 factor:1 | 1 (-2.04589) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13573 HOMO: -6.54434 LUMO: 1.91024 factor:1 | 1 (-1.38966) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90732 HOMO: -6.62869 LUMO: 1.69799 factor:1 | 1 (-1.16125) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99325 HOMO: -6.72393 LUMO: 2.12249 factor:1 | 1 (-1.24718) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24572 HOMO: -6.66407 LUMO: 2.05990 factor:1 | 1 (-1.49965) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30980 HOMO: -7.00149 LUMO: 1.82044 factor:1 | 1 (-1.56373) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36319 HOMO: -7.12122 LUMO: 2.16058 factor:1 | 1 (-1.61712) | 1 | 1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87071 HOMO: -6.63141 LUMO: 2.21229 factor:1 | 1 (-2.12464) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78905 HOMO: -6.37835 LUMO: 2.32113 factor:1 | 1 (-2.04298) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72254 HOMO: -6.99605 LUMO: 2.00548 factor:1 | 1 (-1.97647) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.07673 HOMO: -6.85999 LUMO: 2.39460 factor:1 | 1 (-2.33066) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63321 HOMO: -6.85727 LUMO: 2.48712 factor:1 | 1 (-1.88714) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58042 HOMO: -7.04231 LUMO: 2.40277 factor:1 | 1 (-1.83435) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69609 HOMO: -6.60692 LUMO: 2.26671 factor:1 | 1 (-1.95002) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98478 HOMO: -6.67495 LUMO: 2.14698 factor:1 | 1 (-2.23871) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85495 HOMO: -6.73210 LUMO: 2.06807 factor:1 | 1 (-2.10888) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95052 HOMO: -7.20013 LUMO: 2.02181 factor:1 | 1 (-2.20445) | 1 | 1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84073 HOMO: -7.18653 LUMO: 2.29936 factor:1 | 1 (-1.09466) | 1 | 1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31952 HOMO: -6.92802 LUMO: 2.36195 factor:1 | 1 (-0.57345) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.26948 HOMO: -6.89537 LUMO: 1.78779 factor:1 | 1 (-0.52341) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17901 HOMO: -6.96067 LUMO: 2.31297 factor:1 | 1 (-0.43293) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.12477 HOMO: -6.91441 LUMO: 2.50345 factor:1 | 1 (-0.37870) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.32655 HOMO: -7.17292 LUMO: 2.12521 factor:1 | 1 (-0.58047) | 1 | 1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.91390 HOMO: -6.93618 LUMO: 2.35106 factor:1 | 1 (-1.16783) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76884 HOMO: -6.75931 LUMO: 1.61908 factor:1 | 1 (-1.02277) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77526 HOMO: -6.35930 LUMO: 1.23540 factor:1 | 1 (-1.02919) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13524 HOMO: -6.17971 LUMO: 1.84493 factor:1 | 1 (-1.38917) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81681 HOMO: -6.72665 LUMO: 2.61229 factor:1 | 1 (-1.07074) | -1 | -1 |
| G: -5245.38038 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89733 HOMO: -6.62869 LUMO: 2.28304 factor:1 | 1 (-1.15126) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79986 HOMO: -6.58243 LUMO: 0.28028 factor:1 | 1 (-1.05379) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06621 HOMO: -6.79468 LUMO: 0.14966 factor:1 | 1 (-1.32013) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01722 HOMO: -6.63141 LUMO: 0.31021 factor:1 | 1 (-1.27115) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.95031 HOMO: -6.81101 LUMO: 0.13878 factor:1 | 1 (-1.20424) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96601 HOMO: -6.72665 LUMO: 0.65579 factor:1 | 1 (-1.21994) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.95154 HOMO: -6.53073 LUMO: 0.91430 factor:1 | 1 (-1.20546) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03344 HOMO: -7.19197 LUMO: 1.62996 factor:1 | 1 (-1.28737) | 1 | 1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17734 HOMO: -6.69400 LUMO: 0.84627 factor:1 | 1 (-1.43126) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31285 HOMO: -6.76475 LUMO: 0.51974 factor:1 | 1 (-1.56678) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22139 HOMO: -6.67767 LUMO: 0.52246 factor:1 | 1 (-1.47532) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28896 HOMO: -6.73210 LUMO: 0.94424 factor:1 | 1 (-1.54289) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10253 HOMO: -6.97972 LUMO: 0.60409 factor:1 | 1 (-1.35646) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.02679 HOMO: -7.38517 LUMO: 0.73743 factor:1 | 1 (-2.28072) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84385 HOMO: -6.48992 LUMO: 1.08301 factor:1 | 1 (-2.09778) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.02952 HOMO: -7.18381 LUMO: 1.61908 factor:1 | 1 (-2.28344) | 1 | 1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.27507 HOMO: -6.74842 LUMO: 0.57960 factor:1 | 1 (-2.52900) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04784 HOMO: -6.67495 LUMO: 0.77280 factor:1 | 1 (-1.30177) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18784 HOMO: -6.74570 LUMO: 0.77280 factor:1 | 1 (-1.44177) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17774 HOMO: -6.73754 LUMO: 0.86804 factor:1 | 1 (-1.43167) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03684 HOMO: -6.66135 LUMO: 0.94424 factor:1 | 1 (-2.29076) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87879 HOMO: -6.44638 LUMO: 1.00138 factor:1 | 1 (-2.13272) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.01615 HOMO: -6.65591 LUMO: 1.02043 factor:1 | 1 (-2.27008) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32341 HOMO: -7.17564 LUMO: 0.50069 factor:1 | 1 (-1.57734) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.54125 HOMO: -6.59332 LUMO: 0.79457 factor:1 | -1 (0.20482) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.42895 HOMO: -6.76747 LUMO: 1.73881 factor:1 | -1 (0.31712) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44882 HOMO: -7.00421 LUMO: 1.07485 factor:1 | 1 (-1.70275) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32825 HOMO: -6.94979 LUMO: 1.67894 factor:1 | 1 (-1.58218) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.26835 HOMO: -6.66135 LUMO: 0.47076 factor:1 | -1 (0.47772) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.15885 HOMO: -6.74298 LUMO: 1.85037 factor:1 | -1 (0.58722) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.91473 HOMO: -6.65318 LUMO: 0.95240 factor:1 | 1 (-0.16866) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.88978 HOMO: -6.63958 LUMO: 0.78097 factor:1 | 1 (-0.14370) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46295 HOMO: -6.11712 LUMO: 0.40001 factor:1 | 1 (-1.71688) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31905 HOMO: -7.08312 LUMO: 0.92519 factor:1 | 1 (-1.57298) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77719 HOMO: -6.96067 LUMO: 0.54695 factor:1 | 1 (-1.03112) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.80190 HOMO: -6.74026 LUMO: 0.60137 factor:1 | 1 (-1.05583) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96661 HOMO: -6.74298 LUMO: 0.59593 factor:1 | 1 (-1.22054) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89072 HOMO: -6.93074 LUMO: 0.60681 factor:1 | 1 (-1.14465) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.98073 HOMO: -6.41644 LUMO: 0.35919 factor:1 | 1 (-1.23466) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39261 HOMO: -6.41917 LUMO: 1.73064 factor:1 | 1 (-1.64653) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61337 HOMO: -4.64226 LUMO: -0.87893 factor:1 | 1 (-1.86730) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54322 HOMO: -6.59604 LUMO: 0.90342 factor:1 | 1 (-1.79715) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47988 HOMO: -6.79468 LUMO: 0.50069 factor:1 | 1 (-0.73381) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.61953 HOMO: -7.04503 LUMO: 0.52518 factor:1 | 1 (-0.87346) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40981 HOMO: -6.69400 LUMO: 0.54423 factor:1 | 1 (-0.66374) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21290 HOMO: -6.51713 LUMO: 0.95240 factor:1 | 1 (-1.46683) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76782 HOMO: -6.88176 LUMO: 1.79323 factor:1 | 1 (-2.02175) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76720 HOMO: -6.71849 LUMO: 0.28844 factor:1 | 1 (-2.02113) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76956 HOMO: -6.94979 LUMO: 0.51974 factor:1 | 1 (-2.02349) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84143 HOMO: -6.76203 LUMO: 0.94151 factor:1 | 1 (-2.09536) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54341 HOMO: -6.91169 LUMO: 0.89525 factor:1 | 1 (-1.79734) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70445 HOMO: -6.83006 LUMO: 0.89253 factor:1 | 1 (-1.95838) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79629 HOMO: -7.08857 LUMO: 0.60409 factor:1 | 1 (-2.05021) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68317 HOMO: -6.91713 LUMO: 1.76330 factor:1 | 1 (-1.93710) | -1 | -1 |
| G: -5245.38038 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22166 HOMO: -6.47359 LUMO: 1.56193 factor:1 | 1 (-1.47559) | -1 | -1 |
| G: -5245.38038 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29584 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-1.54977) | -1 | -1 |
| G: -5245.38038 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26904 HOMO: -7.03686 LUMO: 1.97283 factor:1 | 1 (-1.52297) | -1 | -1 |
| G: -5245.38038 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28395 HOMO: -7.00965 LUMO: 1.64629 factor:1 | 1 (-1.53788) | -1 | -1 |
| G: -5245.38038 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03510 HOMO: -7.06952 LUMO: 1.67622 factor:1 | 1 (-1.28903) | 1 | -1 |
| G: -5245.38038 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23935 HOMO: -6.80557 LUMO: 1.70615 factor:1 | 1 (-1.49328) | -1 | -1 |
| G: -5245.38038 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19674 HOMO: -6.80829 LUMO: 1.71704 factor:1 | 1 (-1.45067) | -1 | -1 |
| G: -5245.38038 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25032 HOMO: -7.26544 LUMO: 1.89935 factor:1 | 1 (-1.50425) | 1 | -1 |
| G: -5245.38038 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36921 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-0.62314) | -1 | -1 |
| G: -5245.38038 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49711 HOMO: -7.03686 LUMO: 1.97283 factor:1 | 1 (-0.75103) | -1 | -1 |
| G: -5245.38038 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27190 HOMO: -7.00965 LUMO: 1.64629 factor:1 | 1 (-0.52583) | -1 | -1 |
| G: -5245.38038 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54524 HOMO: -7.06952 LUMO: 1.67622 factor:1 | 1 (-0.79917) | -1 | -1 |
| G: -5245.38038 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41142 HOMO: -6.80557 LUMO: 1.70615 factor:1 | 1 (-0.66535) | -1 | -1 |
| G: -5245.38038 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58878 HOMO: -6.80829 LUMO: 1.71704 factor:1 | 1 (-0.84271) | -1 | -1 |
| G: -5245.38038 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09236 HOMO: -7.26544 LUMO: 1.89935 factor:1 | 1 (-1.34628) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30531 HOMO: -7.00149 LUMO: 1.75241 factor:1 | 1 (-1.55924) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.98068 HOMO: -6.91169 LUMO: 2.07079 factor:1 | 1 (-1.23461) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15029 HOMO: -7.11034 LUMO: 1.76330 factor:1 | 1 (-1.40422) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.92895 HOMO: -6.87360 LUMO: 2.02725 factor:1 | 1 (-1.18288) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18980 HOMO: -7.08584 LUMO: 1.82044 factor:1 | 1 (-1.44373) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.74117 HOMO: -6.90625 LUMO: 1.68166 factor:1 | 1 (-0.99509) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47244 HOMO: -6.71577 LUMO: 1.93201 factor:1 | 1 (-1.72637) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.92003 HOMO: -6.99605 LUMO: 2.08439 factor:1 | 1 (-1.17395) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13761 HOMO: -7.02326 LUMO: 1.97010 factor:1 | 1 (-1.39154) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14471 HOMO: -6.99877 LUMO: 2.15514 factor:1 | 1 (-1.39864) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15094 HOMO: -6.75387 LUMO: 1.95106 factor:1 | 1 (-1.40487) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26972 HOMO: -7.10761 LUMO: 2.06262 factor:1 | 1 (-1.52365) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31584 HOMO: -7.03142 LUMO: 1.91568 factor:1 | 1 (-1.56977) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.16841 HOMO: -6.98788 LUMO: 1.98371 factor:1 | 1 (-1.42234) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99826 HOMO: -6.94707 LUMO: 1.68438 factor:1 | 1 (-1.25219) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10082 HOMO: -6.88176 LUMO: 2.20684 factor:1 | 1 (-1.35475) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02454 HOMO: -6.73210 LUMO: 2.18780 factor:1 | 1 (-1.27847) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17184 HOMO: -6.83822 LUMO: 2.06807 factor:1 | 1 (-1.42577) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13189 HOMO: -6.78924 LUMO: 2.42181 factor:1 | 1 (-1.38582) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19837 HOMO: -6.94707 LUMO: 1.71704 factor:1 | 1 (-1.45230) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08670 HOMO: -6.85183 LUMO: 1.78779 factor:1 | 1 (-1.34062) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41914 HOMO: -6.98788 LUMO: 1.69799 factor:1 | 1 (-1.67306) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08626 HOMO: -6.79468 LUMO: 2.04358 factor:1 | 1 (-1.34019) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01181 HOMO: -6.90081 LUMO: 1.97283 factor:1 | 1 (-1.26574) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25323 HOMO: -6.79468 LUMO: 2.00820 factor:1 | 1 (-1.50716) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40983 HOMO: -7.06408 LUMO: 2.29936 factor:1 | 1 (-1.66376) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37407 HOMO: -6.78924 LUMO: 2.13337 factor:1 | 1 (-1.62800) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38975 HOMO: -6.79468 LUMO: 2.35106 factor:1 | 1 (-1.64368) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.18271 HOMO: -6.82734 LUMO: 2.16603 factor:1 | 1 (-0.43663) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31103 HOMO: -6.79740 LUMO: 2.36739 factor:1 | 1 (-0.56496) | -1 | -1 |
| G: -5245.38038 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70244 HOMO: -7.14027 LUMO: 2.10888 factor:1 | 1 (-0.95637) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.61689 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-0.87082) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.80772 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.06165) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89709 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.15101) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19072 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-1.44465) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02808 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.28201) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08631 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-1.34024) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.98160 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-1.23553) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35315 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.60708) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39419 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.64812) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40717 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.66110) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33806 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.59198) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48923 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.74316) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50472 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.75864) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48323 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-0.73716) | 1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64968 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.90361) | 1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70081 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-0.95474) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77880 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.03273) | 1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96612 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-1.22005) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36946 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.62339) | 1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.30200 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-0.55593) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.16499 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-0.41892) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51977 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.77370) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.24200 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.49593) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.26216 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.51609) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40845 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.66238) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43354 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-0.68747) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72138 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.97531) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63281 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-0.88674) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96264 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.21657) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96457 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-1.21850) | -1 | -1 |
| G: -5245.38038 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22240 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.47633) | 1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33161 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-0.58553) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.25248 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.50640) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21563 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-0.46956) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.30137 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.55530) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27509 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.52902) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29063 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.54455) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36162 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.61555) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42021 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.67413) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07494 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-1.32887) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23078 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-1.48471) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85804 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-1.11197) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06621 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.32013) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41723 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.67116) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28381 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.53774) | 1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43310 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.68702) | 1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81172 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.06565) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81689 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.07082) | 1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56805 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.82197) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.68252 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.93645) | 1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85243 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.10636) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90310 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-1.15703) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04833 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-1.30226) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.80647 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-1.06040) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.94389 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-1.19782) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89788 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-1.15180) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67768 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-0.93161) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75605 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-1.00998) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55806 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-0.81199) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47811 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.73204) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46573 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.71966) | -1 | -1 |
| G: -5245.38038 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44559 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.69952) | 1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.25163 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-0.50556) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.23008 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.48401) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48665 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.74058) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52145 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-1.77538) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36850 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.62242) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52308 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-1.77701) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88098 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-1.13491) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75110 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.00503) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63602 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.88995) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71096 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.96489) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50135 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.75528) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.20881 HOMO: -6.62869 LUMO: 1.69527 factor:1 | -1 (0.53726) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72946 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-0.98339) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.61302 HOMO: -7.07768 LUMO: 1.27621 factor:1 | -1 (1.13305) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.68662 HOMO: -7.06135 LUMO: 1.55105 factor:1 | -1 (1.05945) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.62869 HOMO: -6.94162 LUMO: 1.64629 factor:1 | -1 (1.11738) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.54417 HOMO: -7.07224 LUMO: 1.65445 factor:1 | -1 (1.20190) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.70287 HOMO: -6.68584 LUMO: 1.91296 factor:1 | -1 (1.04320) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.40363 HOMO: -7.09129 LUMO: 1.73609 factor:1 | -1 (1.34245) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27002 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.52395) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81006 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-2.06398) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47536 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-1.72928) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72029 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-1.97421) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22781 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-1.48174) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12071 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-1.37464) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.16762 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.42155) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52066 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-1.77459) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13638 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-1.39031) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58198 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.83591) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86013 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-1.11406) | -1 | -1 |
| G: -5245.38038 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38110 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.63503) | -1 | -1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56549 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-0.81942) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72481 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.97874) | -1 | -1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04346 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.29738) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.95823 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-1.21216) | -1 | -1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79589 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.04982) | -1 | -1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.92215 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-1.17608) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24370 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-1.49763) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33342 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.58735) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35323 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-1.60716) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24128 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-1.49521) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25750 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-1.51143) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.16613 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.42005) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36186 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.61578) | -1 | -1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34602 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.59995) | -1 | -1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21021 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.46414) | -1 | -1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18044 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.43437) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07755 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.33148) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19998 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-1.45390) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04759 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.30152) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14819 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.40212) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26166 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-2.51558) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50104 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-1.75497) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27377 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-1.52770) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18871 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-1.44264) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69819 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-1.95212) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58692 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.84085) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63462 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-1.88855) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42580 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-1.67973) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07320 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.32713) | -1 | -1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.91597 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-1.16990) | 1 | 1 |
| G: -5245.38038 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.94944 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.20337) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03595 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.28987) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90166 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.15559) | -1 | -1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71409 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-0.96802) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65510 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.90902) | -1 | -1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24006 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.49399) | -1 | -1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.98999 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-1.24391) | -1 | -1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20259 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-1.45652) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13241 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.38634) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20395 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-1.45788) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04411 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-1.29804) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21445 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-1.46838) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26985 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-2.52377) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.53766 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-2.79159) | -1 | -1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.17197 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-2.42590) | -1 | -1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13077 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-2.38470) | -1 | -1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.21774 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-2.47166) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56260 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.81652) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68657 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-1.94050) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71297 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.96689) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60668 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.86061) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73188 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-1.98581) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78472 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-2.03865) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50420 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-1.75813) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30879 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-1.56272) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34300 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-1.59693) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31312 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.56705) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14430 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-1.39823) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03464 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-1.28857) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.40898 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-2.66291) | -1 | -1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.23262 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-2.48655) | 1 | 1 |
| G: -5245.38038 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.21208 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-2.46600) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86543 HOMO: -7.06135 LUMO: 0.75376 factor:1 | 1 (-2.11936) | 1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31529 HOMO: -5.10213 LUMO: 0.77825 factor:1 | 1 (-2.56922) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.21115 HOMO: -5.84228 LUMO: 0.50341 factor:1 | 1 (-2.46508) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.76847 HOMO: -5.39874 LUMO: 0.68028 factor:1 | 1 (-3.02240) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.82719 HOMO: -5.16744 LUMO: 1.14832 factor:1 | 1 (-3.08112) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57908 HOMO: -5.80963 LUMO: 0.35647 factor:1 | 1 (-2.83300) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55807 HOMO: -5.02322 LUMO: 1.07213 factor:1 | 1 (-2.81200) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.76692 HOMO: -5.80963 LUMO: 0.56328 factor:1 | 1 (-3.02084) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.39050 HOMO: -5.45316 LUMO: 0.78369 factor:1 | 1 (-2.64443) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.42313 HOMO: -5.25452 LUMO: 0.82178 factor:1 | 1 (-2.67706) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.33404 HOMO: -5.21370 LUMO: 1.03947 factor:1 | 1 (-2.58797) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.18476 HOMO: -6.04365 LUMO: 0.31837 factor:1 | 1 (-2.43868) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.34862 HOMO: -5.86405 LUMO: 0.55511 factor:1 | 1 (-2.60255) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43971 HOMO: -5.64908 LUMO: 0.71022 factor:1 | 1 (-1.69364) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.17667 HOMO: -5.94297 LUMO: 0.68301 factor:1 | 1 (-2.43060) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95670 HOMO: -6.01916 LUMO: 0.56328 factor:1 | 1 (-2.21063) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.10192 HOMO: -6.05181 LUMO: 0.35103 factor:1 | 1 (-2.35585) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59533 HOMO: -6.08447 LUMO: 0.48436 factor:1 | 1 (-1.84926) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85947 HOMO: -5.86950 LUMO: 0.36735 factor:1 | 1 (-2.11340) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48102 HOMO: -5.33615 LUMO: 0.65852 factor:1 | 1 (-1.73494) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98644 HOMO: -5.36064 LUMO: 0.86804 factor:1 | 1 (-2.24037) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65530 HOMO: -5.74160 LUMO: 0.64491 factor:1 | 1 (-1.90923) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03411 HOMO: -5.23003 LUMO: 0.66124 factor:1 | 1 (-2.28804) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91735 HOMO: -5.77698 LUMO: 0.84083 factor:1 | 1 (-2.17128) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13942 HOMO: -5.60555 LUMO: 0.84355 factor:1 | 1 (-2.39335) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84693 HOMO: -7.11578 LUMO: -1.62452 factor:1 | 1 (-2.10086) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.04837 HOMO: -7.23279 LUMO: -1.63813 factor:1 | 1 (-2.30230) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85433 HOMO: -6.68312 LUMO: -0.88709 factor:1 | 1 (-2.10826) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83694 HOMO: -6.99333 LUMO: -0.88709 factor:1 | 1 (-2.09087) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.06699 HOMO: -7.40694 LUMO: 0.11973 factor:1 | 1 (-2.32091) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64779 HOMO: -6.74026 LUMO: -0.72927 factor:1 | 1 (-1.90172) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60540 HOMO: -6.67223 LUMO: -0.70750 factor:1 | 1 (-1.85933) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57857 HOMO: -7.06952 LUMO: -1.40139 factor:1 | 1 (-1.83250) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45258 HOMO: -7.21374 LUMO: -1.13199 factor:1 | 1 (-1.70651) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64072 HOMO: -6.54706 LUMO: -1.34424 factor:1 | 1 (-1.89465) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69454 HOMO: -7.51851 LUMO: -1.05852 factor:1 | 1 (-1.94847) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91637 HOMO: -7.07224 LUMO: -1.89391 factor:1 | 1 (-2.17030) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31665 HOMO: -6.65863 LUMO: -0.46804 factor:1 | 1 (-2.57058) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.05591 HOMO: -7.24367 LUMO: 0.29388 factor:1 | 1 (-2.30984) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13825 HOMO: -7.02326 LUMO: -0.87893 factor:1 | 1 (-2.39218) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.11515 HOMO: -6.88176 LUMO: 0.71566 factor:1 | 1 (-2.36908) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.24185 HOMO: -6.46543 LUMO: 1.01498 factor:1 | 1 (-2.49577) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.07727 HOMO: -6.30760 LUMO: 0.17687 factor:1 | 1 (-2.33120) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.07365 HOMO: -6.73210 LUMO: -1.06941 factor:1 | 1 (-2.32758) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.34261 HOMO: -6.83550 LUMO: -0.75920 factor:1 | 1 (-2.59654) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.46022 HOMO: -6.94707 LUMO: 0.42178 factor:1 | 1 (-2.71415) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30577 HOMO: -6.77019 LUMO: -0.38096 factor:1 | 1 (-2.55969) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20432 HOMO: -7.34163 LUMO: 0.35103 factor:1 | 1 (-2.45825) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.35192 HOMO: -6.87632 LUMO: -0.87349 factor:1 | 1 (-2.60584) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55562 HOMO: -7.06952 LUMO: -1.47214 factor:1 | 1 (-2.80955) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48103 HOMO: -6.58788 LUMO: -0.37824 factor:1 | 1 (-2.73496) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44444 HOMO: -6.92802 LUMO: -1.24900 factor:1 | 1 (-1.69837) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.91276 HOMO: -7.01237 LUMO: -1.31975 factor:1 | 1 (-1.16669) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49156 HOMO: -6.74842 LUMO: 0.45987 factor:1 | 1 (-0.74548) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44143 HOMO: -6.53890 LUMO: 0.94424 factor:1 | 1 (-0.69536) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76982 HOMO: -6.52257 LUMO: -0.66940 factor:1 | 1 (-1.02375) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57196 HOMO: -6.56883 LUMO: -1.48302 factor:1 | 1 (-1.82588) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56877 HOMO: -7.21646 LUMO: 0.13061 factor:1 | 1 (-1.82270) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52608 HOMO: -6.62597 LUMO: -0.64763 factor:1 | 1 (-1.78001) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45623 HOMO: -7.38789 LUMO: 0.31021 factor:1 | 1 (-1.71015) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63653 HOMO: -6.74570 LUMO: -0.70750 factor:1 | 1 (-1.89046) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.29221 HOMO: -6.95251 LUMO: -1.25989 factor:1 | 1 (-2.54614) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26838 HOMO: -7.13483 LUMO: -0.76736 factor:1 | 1 (-2.52231) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08073 HOMO: -6.93618 LUMO: -1.24628 factor:1 | 1 (-2.33466) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45818 HOMO: -7.03686 LUMO: 0.26395 factor:1 | 1 (-2.71210) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.91865 HOMO: -6.52257 LUMO: -0.84355 factor:1 | 1 (-3.17258) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.78273 HOMO: -6.83278 LUMO: -0.49525 factor:1 | 1 (-3.03665) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.93253 HOMO: -7.18381 LUMO: -1.64629 factor:1 | 1 (-3.18645) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75732 HOMO: -6.74842 LUMO: -0.81090 factor:1 | 1 (-2.01125) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60303 HOMO: -7.09401 LUMO: -0.92519 factor:1 | 1 (-1.85696) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.61753 HOMO: -7.20285 LUMO: -0.81634 factor:1 | 1 (-2.87145) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52464 HOMO: -6.72665 LUMO: 0.77008 factor:1 | 1 (-1.77856) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57336 HOMO: -6.80829 LUMO: 0.86532 factor:1 | 1 (-2.82729) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67109 HOMO: -6.20964 LUMO: 0.99866 factor:1 | 1 (-1.92502) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55159 HOMO: -6.52801 LUMO: 1.07757 factor:1 | 1 (-2.80552) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.36479 HOMO: -6.74298 LUMO: -0.67756 factor:1 | 1 (-2.61871) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.50568 HOMO: -7.43959 LUMO: 0.03265 factor:1 | 1 (-3.75961) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.02461 HOMO: -6.46815 LUMO: -0.29933 factor:1 | 1 (-3.27854) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.02488 HOMO: -6.70489 LUMO: -0.97145 factor:1 | 1 (-3.27881) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.88278 HOMO: -6.30216 LUMO: -1.39322 factor:1 | 1 (-3.13671) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.18638 HOMO: -7.01782 LUMO: -1.07485 factor:1 | 1 (-3.44031) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.90686 HOMO: -6.93074 LUMO: 0.25851 factor:1 | 1 (-4.16078) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.25825 HOMO: -7.07224 LUMO: 0.09524 factor:1 | 1 (-3.51217) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.76979 HOMO: -6.62325 LUMO: -0.45443 factor:1 | 1 (-4.02372) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.14175 HOMO: -7.09945 LUMO: -1.20274 factor:1 | 1 (-3.39568) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.06167 HOMO: -6.56067 LUMO: -1.39322 factor:1 | 1 (-3.31560) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.99634 HOMO: -6.75387 LUMO: -0.72654 factor:1 | 1 (-3.25026) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.87037 HOMO: -6.28583 LUMO: -2.35651 factor:1 | 1 (-4.12429) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.99290 HOMO: -6.55522 LUMO: -1.33608 factor:1 | 1 (-4.24683) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.21944 HOMO: -7.19741 LUMO: -0.93607 factor:1 | 1 (-3.47337) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.07008 HOMO: -6.39740 LUMO: -1.14832 factor:1 | 1 (-3.32401) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.35219 HOMO: -7.11850 LUMO: -0.97417 factor:1 | 1 (-2.60612) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.36313 HOMO: -6.57699 LUMO: -1.14016 factor:1 | 1 (-2.61706) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.36775 HOMO: -6.57699 LUMO: -1.31975 factor:1 | 1 (-2.62168) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49018 HOMO: -6.69128 LUMO: -0.76736 factor:1 | 1 (-2.74411) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.41302 HOMO: -7.25728 LUMO: 0.29660 factor:1 | 1 (-3.66695) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01691 HOMO: -6.37019 LUMO: -0.95240 factor:1 | 1 (-3.27084) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.38109 HOMO: -6.48447 LUMO: -0.55511 factor:1 | 1 (-2.63501) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.12875 HOMO: -6.37291 LUMO: -0.78641 factor:1 | 1 (-3.38267) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.23240 HOMO: -6.65863 LUMO: -0.69933 factor:1 | 1 (-2.48633) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49505 HOMO: -6.44638 LUMO: -0.16055 factor:1 | 1 (-2.74898) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.39181 HOMO: -6.41917 LUMO: -0.20136 factor:1 | 1 (-2.64574) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.53203 HOMO: -7.33347 LUMO: 0.12789 factor:1 | 1 (-2.78596) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.28690 HOMO: -6.70489 LUMO: -0.52518 factor:1 | 1 (-3.54083) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73528 HOMO: -7.25183 LUMO: 0.32109 factor:1 | 1 (-1.98921) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62047 HOMO: -7.29265 LUMO: 0.28028 factor:1 | 1 (-1.87440) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58834 HOMO: -6.57155 LUMO: -0.51702 factor:1 | 1 (-1.84227) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.47246 HOMO: -7.08040 LUMO: 0.39729 factor:1 | 1 (-2.72639) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66477 HOMO: -6.24501 LUMO: -0.44627 factor:1 | 1 (-1.91870) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47413 HOMO: -6.73754 LUMO: -0.45443 factor:1 | 1 (-1.72806) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53133 HOMO: -6.24501 LUMO: 0.38096 factor:1 | 1 (-1.78526) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.42974 HOMO: -6.86815 LUMO: -0.91974 factor:1 | 1 (-2.68367) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.95087 HOMO: -7.40150 LUMO: 0.36191 factor:1 | 1 (-3.20479) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.28938 HOMO: -6.44094 LUMO: -0.64219 factor:1 | 1 (-2.54331) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.58074 HOMO: -6.69944 LUMO: -0.80001 factor:1 | 1 (-2.83466) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.10107 HOMO: -6.61509 LUMO: -0.70750 factor:1 | 1 (-3.35500) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.32834 HOMO: -7.52123 LUMO: 0.06803 factor:1 | 1 (-3.58227) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60046 HOMO: -7.34163 LUMO: 0.30477 factor:1 | 1 (-2.85439) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.35009 HOMO: -6.68584 LUMO: -0.78641 factor:1 | 1 (-2.60402) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.46724 HOMO: -6.53890 LUMO: -0.50885 factor:1 | 1 (-2.72117) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68444 HOMO: -6.75659 LUMO: -0.68845 factor:1 | 1 (-2.93837) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.46144 HOMO: -7.08857 LUMO: 0.43266 factor:1 | 1 (-2.71537) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.75995 HOMO: -6.28583 LUMO: -0.46804 factor:1 | 1 (-3.01388) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.02356 HOMO: -6.50080 LUMO: -0.24762 factor:1 | 1 (-2.27748) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.69726 HOMO: -6.45454 LUMO: -0.58504 factor:1 | 1 (-2.95118) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.10592 HOMO: -7.20558 LUMO: 0.20953 factor:1 | 1 (-2.35985) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.37279 HOMO: -6.35930 LUMO: -0.20681 factor:1 | 1 (-2.62672) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.11900 HOMO: -6.36202 LUMO: -0.14422 factor:1 | 1 (-3.37293) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.13228 HOMO: -6.20692 LUMO: 1.97827 factor:1 | 1 (-3.38621) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.04570 HOMO: -6.48719 LUMO: 1.74153 factor:1 | 1 (-3.29963) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.93533 HOMO: -6.84638 LUMO: 1.88575 factor:1 | 1 (-3.18926) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.64946 HOMO: -5.90759 LUMO: 2.00820 factor:1 | 1 (-3.90339) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.03865 HOMO: -6.56339 LUMO: 1.99732 factor:1 | 1 (-3.29258) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.08608 HOMO: -6.20692 LUMO: 1.75241 factor:1 | 1 (-3.34001) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.44754 HOMO: -6.16882 LUMO: 1.94017 factor:1 | 1 (-2.70146) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.53510 HOMO: -6.80829 LUMO: 1.78507 factor:1 | 1 (-2.78903) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.36422 HOMO: -6.58243 LUMO: 1.78235 factor:1 | 1 (-2.61814) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.98251 HOMO: -5.85045 LUMO: 1.82316 factor:1 | 1 (-3.23644) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.09636 HOMO: -5.93752 LUMO: 1.56465 factor:1 | 1 (-3.35029) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.23925 HOMO: -6.59604 LUMO: -0.53334 factor:1 | 1 (-3.49318) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.07816 HOMO: -7.06135 LUMO: 0.29660 factor:1 | 1 (-3.33209) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.89649 HOMO: -6.50352 LUMO: 1.61908 factor:1 | 1 (-4.15042) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.52116 HOMO: -6.68040 LUMO: -0.60681 factor:1 | 1 (-3.77509) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48261 HOMO: -6.93618 LUMO: -1.09662 factor:1 | 1 (-2.73654) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.35300 HOMO: -6.72121 LUMO: -1.14016 factor:1 | 1 (-2.60693) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51442 HOMO: -7.12394 LUMO: -1.24900 factor:1 | 1 (-2.76835) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.29319 HOMO: -6.71305 LUMO: -0.71566 factor:1 | 1 (-2.54712) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.14023 HOMO: -7.09401 LUMO: -0.86532 factor:1 | 1 (-3.39416) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.37445 HOMO: -7.08584 LUMO: -0.92519 factor:1 | 1 (-2.62837) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.23284 HOMO: -7.05591 LUMO: 0.11973 factor:1 | 1 (-2.48677) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14884 HOMO: -7.14843 LUMO: -1.58370 factor:1 | 1 (-2.40277) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.98159 HOMO: -7.36884 LUMO: -1.97010 factor:1 | 1 (-3.23552) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.95253 HOMO: -6.81373 LUMO: -1.72248 factor:1 | 1 (-3.20645) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.02393 HOMO: -6.87360 LUMO: -1.03947 factor:1 | 1 (-3.27786) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57214 HOMO: -7.02870 LUMO: -0.87349 factor:1 | 1 (-2.82607) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.39034 HOMO: -7.16476 LUMO: -1.18097 factor:1 | 1 (-2.64427) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20710 HOMO: -7.51851 LUMO: 0.07891 factor:1 | 1 (-2.46102) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.43973 HOMO: -7.04231 LUMO: -0.83539 factor:1 | 1 (-2.69366) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15259 HOMO: -6.83278 LUMO: -0.60137 factor:1 | 1 (-2.40652) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.10729 HOMO: -6.89809 LUMO: -1.19186 factor:1 | 1 (-2.36121) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.69924 HOMO: -7.16476 LUMO: -0.79185 factor:1 | 1 (-2.95317) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64259 HOMO: -6.97156 LUMO: -1.25444 factor:1 | 1 (-2.89652) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60289 HOMO: -6.84366 LUMO: -0.88437 factor:1 | 1 (-2.85681) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.37488 HOMO: -6.91986 LUMO: -1.12655 factor:1 | 1 (-2.62881) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.19711 HOMO: -6.49536 LUMO: -0.29660 factor:1 | 1 (-2.45104) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00723 HOMO: -6.74842 LUMO: 0.42450 factor:1 | 1 (-2.26116) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.24527 HOMO: -7.34435 LUMO: 0.32109 factor:1 | 1 (-2.49920) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.42294 HOMO: -7.16476 LUMO: 0.28572 factor:1 | 1 (-2.67687) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.39178 HOMO: -6.74298 LUMO: -0.43538 factor:1 | 1 (-2.64571) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20223 HOMO: -7.19469 LUMO: -1.61091 factor:1 | 1 (-2.45615) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.98023 HOMO: -7.35252 LUMO: -1.78235 factor:1 | 1 (-3.23415) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.06300 HOMO: -7.25456 LUMO: -1.66806 factor:1 | 1 (-3.31693) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13341 HOMO: -7.54844 LUMO: -1.07213 factor:1 | 1 (-2.38734) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.94531 HOMO: -7.21918 LUMO: -1.55377 factor:1 | 1 (-3.19924) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.53229 HOMO: -7.01782 LUMO: -1.60547 factor:1 | 1 (-3.78622) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45782 HOMO: -7.21646 LUMO: -1.53472 factor:1 | 1 (-2.71175) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.42277 HOMO: -6.73754 LUMO: -1.37417 factor:1 | 1 (-2.67670) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.39815 HOMO: -6.78924 LUMO: 0.66396 factor:1 | 1 (-2.65208) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.35213 HOMO: -6.82734 LUMO: 0.61226 factor:1 | 1 (-2.60606) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.07291 HOMO: -6.74026 LUMO: 0.65579 factor:1 | 1 (-3.32684) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.23009 HOMO: -7.10489 LUMO: -1.30887 factor:1 | 1 (-2.48402) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.18734 HOMO: -7.05047 LUMO: 0.42722 factor:1 | 1 (-2.44127) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.28166 HOMO: -6.61237 LUMO: 1.30887 factor:1 | 1 (-2.53558) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98892 HOMO: -7.05863 LUMO: 0.59049 factor:1 | 1 (-2.24284) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.73209 HOMO: -6.26406 LUMO: 0.78641 factor:1 | 1 (-2.98601) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.98159 HOMO: -6.70489 LUMO: 0.67756 factor:1 | 1 (-3.23552) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.25017 HOMO: -6.78652 LUMO: -0.94968 factor:1 | 1 (-2.50410) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.25659 HOMO: -6.36202 LUMO: -0.94424 factor:1 | 1 (-2.51052) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.12652 HOMO: -6.81645 LUMO: -1.09934 factor:1 | 1 (-3.38044) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15627 HOMO: -7.07224 LUMO: 0.85988 factor:1 | 1 (-2.41019) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.29978 HOMO: -7.02326 LUMO: 1.10206 factor:1 | 1 (-2.55371) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.29224 HOMO: -6.71305 LUMO: 0.84627 factor:1 | 1 (-2.54617) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.94820 HOMO: -7.27360 LUMO: 0.88165 factor:1 | 1 (-3.20213) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.11062 HOMO: -6.84911 LUMO: 0.59865 factor:1 | 1 (-3.36455) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.38068 HOMO: -6.75114 LUMO: -2.49801 factor:1 | 1 (-2.63461) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.34117 HOMO: -6.97156 LUMO: 0.53606 factor:1 | 1 (-2.59510) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.16855 HOMO: -6.54434 LUMO: 0.73199 factor:1 | 1 (-1.42248) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15559 HOMO: -6.21236 LUMO: 0.99866 factor:1 | 1 (-2.40951) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14870 HOMO: -6.34025 LUMO: 0.50341 factor:1 | 1 (-2.40263) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46817 HOMO: -6.59876 LUMO: -0.69389 factor:1 | 1 (-1.72210) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26256 HOMO: -6.54978 LUMO: -1.00682 factor:1 | 1 (-1.51649) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42812 HOMO: -6.82462 LUMO: -0.98777 factor:1 | 1 (-1.68204) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20104 HOMO: -6.85455 LUMO: -0.68573 factor:1 | 1 (-1.45497) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34251 HOMO: -7.55388 LUMO: -0.03265 factor:1 | 1 (-1.59644) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39783 HOMO: -6.77019 LUMO: -0.71838 factor:1 | 1 (-1.65176) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31230 HOMO: -6.84911 LUMO: -1.25444 factor:1 | 1 (-1.56623) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30305 HOMO: -6.95251 LUMO: -1.03675 factor:1 | 1 (-1.55698) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10207 HOMO: -6.80829 LUMO: -0.77280 factor:1 | 1 (-1.35600) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.06132 HOMO: -6.94162 LUMO: -0.94151 factor:1 | 1 (-3.31524) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93049 HOMO: -6.89809 LUMO: -0.90886 factor:1 | 1 (-2.18442) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88012 HOMO: -6.85183 LUMO: -0.88981 factor:1 | 1 (-2.13405) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88004 HOMO: -6.51985 LUMO: -0.84627 factor:1 | 1 (-2.13397) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15768 HOMO: -6.83278 LUMO: -1.08029 factor:1 | 1 (-2.41161) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99754 HOMO: -6.91986 LUMO: 0.66396 factor:1 | 1 (-2.25147) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.18922 HOMO: -6.94162 LUMO: 0.50885 factor:1 | 1 (-2.44315) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13774 HOMO: -6.94435 LUMO: 0.80546 factor:1 | 1 (-2.39166) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14938 HOMO: -6.74298 LUMO: -0.81634 factor:1 | 1 (-2.40331) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.47015 HOMO: -7.04503 LUMO: 1.15921 factor:1 | 1 (-2.72408) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62351 HOMO: -6.76475 LUMO: 0.75920 factor:1 | 1 (-2.87744) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.77179 HOMO: -7.05047 LUMO: 0.68845 factor:1 | 1 (-3.02572) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65464 HOMO: -7.12666 LUMO: 0.60681 factor:1 | 1 (-2.90857) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26873 HOMO: -6.90897 LUMO: -1.22723 factor:1 | 1 (-2.52266) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13926 HOMO: -7.10761 LUMO: 0.58232 factor:1 | 1 (-2.39319) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.22367 HOMO: -6.57427 LUMO: 0.71294 factor:1 | 1 (-2.47760) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31227 HOMO: -6.22597 LUMO: 0.99322 factor:1 | 1 (-2.56620) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.27458 HOMO: -6.83550 LUMO: -0.77825 factor:1 | 1 (-2.52851) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.53878 HOMO: -7.14843 LUMO: 0.44627 factor:1 | 1 (-2.79270) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62199 HOMO: -7.08040 LUMO: 0.78913 factor:1 | 1 (-2.87592) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.53905 HOMO: -6.81373 LUMO: -0.93879 factor:1 | 1 (-2.79298) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81822 HOMO: -6.95251 LUMO: 0.22585 factor:1 | 1 (-2.07215) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77571 HOMO: -7.13483 LUMO: -1.25444 factor:1 | 1 (-2.02964) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92881 HOMO: -6.37835 LUMO: -1.54289 factor:1 | 1 (-2.18273) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51733 HOMO: -6.53617 LUMO: -1.43948 factor:1 | 1 (-2.77126) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85457 HOMO: -6.38379 LUMO: 0.16055 factor:1 | 1 (-2.10850) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99871 HOMO: -6.53617 LUMO: 0.15783 factor:1 | 1 (-2.25264) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31266 HOMO: -6.79740 LUMO: -0.17960 factor:1 | 1 (-1.56659) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38607 HOMO: -6.26678 LUMO: -0.41361 factor:1 | 1 (-1.64000) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.17967 HOMO: -6.35658 LUMO: -0.24218 factor:1 | 1 (-2.43360) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03063 HOMO: -6.48175 LUMO: -0.71566 factor:1 | 1 (-2.28456) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20179 HOMO: -6.21508 LUMO: -0.40001 factor:1 | 1 (-2.45572) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41761 HOMO: -6.51985 LUMO: -0.32654 factor:1 | 1 (-1.67154) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26107 HOMO: -6.45182 LUMO: -0.66396 factor:1 | 1 (-1.51499) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29413 HOMO: -6.51441 LUMO: -0.65307 factor:1 | 1 (-1.54806) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32316 HOMO: -6.57971 LUMO: -0.92519 factor:1 | 1 (-1.57709) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15048 HOMO: -6.67223 LUMO: -0.58232 factor:1 | 1 (-1.40441) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27462 HOMO: -6.10351 LUMO: -0.45987 factor:1 | 1 (-1.52855) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59506 HOMO: -6.13889 LUMO: -0.50341 factor:1 | 1 (-1.84899) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59620 HOMO: -6.63141 LUMO: -0.28300 factor:1 | 1 (-1.85013) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31285 HOMO: -6.37563 LUMO: -0.22858 factor:1 | 1 (-1.56678) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08114 HOMO: -6.37019 LUMO: 0.11429 factor:1 | 1 (-2.33506) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86015 HOMO: -6.23957 LUMO: 0.28844 factor:1 | 1 (-2.11408) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54234 HOMO: -6.41372 LUMO: -0.53879 factor:1 | 1 (-2.79627) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.66613 HOMO: -7.06680 LUMO: 0.32654 factor:1 | 1 (-2.92005) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.58400 HOMO: -6.50896 LUMO: -0.73743 factor:1 | 1 (-2.83793) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54210 HOMO: -6.42189 LUMO: -0.28572 factor:1 | 1 (-2.79602) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08786 HOMO: -6.79740 LUMO: -0.25851 factor:1 | 1 (-2.34178) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13812 HOMO: -6.32393 LUMO: 0.17960 factor:1 | 1 (-2.39204) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.19929 HOMO: -6.65046 LUMO: 0.03537 factor:1 | 1 (-2.45322) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03719 HOMO: -6.60148 LUMO: 0.07619 factor:1 | 1 (-2.29112) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12446 HOMO: -6.57971 LUMO: 0.11429 factor:1 | 1 (-2.37838) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.18076 HOMO: -6.88448 LUMO: -1.21907 factor:1 | 1 (-2.43468) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.40796 HOMO: -6.97700 LUMO: 0.36463 factor:1 | 1 (-3.66189) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.04240 HOMO: -6.73210 LUMO: -0.84083 factor:1 | 1 (-3.29633) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54183 HOMO: -6.21236 LUMO: -0.68845 factor:1 | 1 (-1.79576) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24313 HOMO: -6.35658 LUMO: -0.82995 factor:1 | 1 (-1.49706) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49802 HOMO: -6.75114 LUMO: -0.94424 factor:1 | 1 (-1.75195) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23932 HOMO: -6.74026 LUMO: -1.46125 factor:1 | 1 (-1.49325) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26286 HOMO: -7.06952 LUMO: 0.91974 factor:1 | 1 (-1.51679) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26308 HOMO: -7.08857 LUMO: 0.74559 factor:1 | 1 (-1.51701) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15557 HOMO: -6.74298 LUMO: 1.03131 factor:1 | 1 (-1.40950) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91876 HOMO: -6.74842 LUMO: -1.77962 factor:1 | 1 (-2.17269) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00949 HOMO: -6.82462 LUMO: -1.61908 factor:1 | 1 (-2.26342) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.18266 HOMO: -7.17020 LUMO: -1.02043 factor:1 | 1 (-2.43659) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.01945 HOMO: -6.26406 LUMO: -0.96328 factor:1 | 1 (-2.27338) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03115 HOMO: -6.50896 LUMO: -0.38640 factor:1 | 1 (-2.28508) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79525 HOMO: -7.27632 LUMO: -1.17553 factor:1 | 1 (-2.04918) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80600 HOMO: -6.54162 LUMO: -1.36873 factor:1 | 1 (-2.05993) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00040 HOMO: -6.42733 LUMO: -1.15648 factor:1 | 1 (-2.25433) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86905 HOMO: -6.73754 LUMO: -2.58780 factor:1 | 1 (-2.12298) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.29366 HOMO: -7.20285 LUMO: 0.75103 factor:1 | 1 (-2.54758) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79640 HOMO: -6.98788 LUMO: 0.34831 factor:1 | 1 (-2.05032) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.18130 HOMO: -6.80013 LUMO: -1.11567 factor:1 | 1 (-2.43523) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14225 HOMO: -6.67767 LUMO: -0.82450 factor:1 | 1 (-2.39618) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.05207 HOMO: -6.84911 LUMO: -0.21497 factor:1 | 1 (-2.30600) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89038 HOMO: -6.23141 LUMO: 0.21769 factor:1 | 1 (-2.14431) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.25287 HOMO: -6.68312 LUMO: 0.16327 factor:1 | 1 (-2.50679) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.43841 HOMO: -7.04503 LUMO: -1.04220 factor:1 | 1 (-3.69234) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14612 HOMO: -6.67495 LUMO: -0.71294 factor:1 | 1 (-2.40004) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.02462 HOMO: -6.70216 LUMO: -0.55239 factor:1 | 1 (-2.27855) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90793 HOMO: -6.60420 LUMO: -0.71294 factor:1 | 1 (-2.16186) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89199 HOMO: -7.40694 LUMO: 0.11973 factor:1 | 1 (-2.14592) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.90012 HOMO: -6.58788 LUMO: -0.29116 factor:1 | 1 (-3.15404) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26563 HOMO: -6.63686 LUMO: -0.32654 factor:1 | 1 (-2.51956) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90418 HOMO: -6.85183 LUMO: -0.95512 factor:1 | 1 (-2.15811) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89585 HOMO: -6.82189 LUMO: -0.88165 factor:1 | 1 (-2.14978) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.01098 HOMO: -6.97428 LUMO: -1.03947 factor:1 | 1 (-2.26491) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30846 HOMO: -6.51441 LUMO: -0.05714 factor:1 | 1 (-2.56239) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.17882 HOMO: -6.61509 LUMO: -0.77008 factor:1 | 1 (-2.43275) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.41539 HOMO: -7.36340 LUMO: 0.29116 factor:1 | 1 (-3.66932) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15510 HOMO: -6.64230 LUMO: -0.79185 factor:1 | 1 (-2.40902) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20941 HOMO: -6.56883 LUMO: -1.03403 factor:1 | 1 (-2.46334) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.24272 HOMO: -6.69400 LUMO: -0.77825 factor:1 | 1 (-2.49664) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56553 HOMO: -6.37019 LUMO: -0.79185 factor:1 | 1 (-2.81945) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.42177 HOMO: -6.49808 LUMO: -0.94424 factor:1 | 1 (-2.67570) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13910 HOMO: -6.91713 LUMO: -0.75376 factor:1 | 1 (-2.39302) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18806 HOMO: -7.13755 LUMO: 0.41361 factor:1 | 1 (-1.44199) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33233 HOMO: -7.12122 LUMO: 0.39457 factor:1 | 1 (-1.58626) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67068 HOMO: -6.59332 LUMO: -0.57144 factor:1 | 1 (-1.92461) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.18448 HOMO: -6.62325 LUMO: -0.66940 factor:1 | 1 (-2.43841) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.34607 HOMO: -6.90897 LUMO: -0.08708 factor:1 | 1 (-2.59999) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76420 HOMO: -6.65591 LUMO: -0.81090 factor:1 | 1 (-2.01813) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63430 HOMO: -6.65318 LUMO: -0.94696 factor:1 | 1 (-1.88823) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86470 HOMO: -6.96067 LUMO: -1.03675 factor:1 | 1 (-2.11862) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49488 HOMO: -6.23141 LUMO: -0.66396 factor:1 | 1 (-2.74881) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.04138 HOMO: -6.52529 LUMO: -0.78369 factor:1 | 1 (-2.29531) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.05319 HOMO: -6.39468 LUMO: -0.40817 factor:1 | 1 (-2.30712) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93634 HOMO: -6.76203 LUMO: -0.20409 factor:1 | 1 (-2.19027) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.37812 HOMO: -6.96611 LUMO: -0.90342 factor:1 | 1 (-2.63205) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.73873 HOMO: -6.54706 LUMO: -0.87893 factor:1 | 1 (-2.99265) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42316 HOMO: -7.24367 LUMO: -0.97689 factor:1 | 1 (-1.67709) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29952 HOMO: -6.61781 LUMO: 1.43404 factor:1 | 1 (-1.55344) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.04269 HOMO: -6.17971 LUMO: 1.79867 factor:1 | 1 (-2.29661) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49295 HOMO: -5.73344 LUMO: 2.13609 factor:1 | 1 (-2.74688) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49872 HOMO: -6.72121 LUMO: 2.06807 factor:1 | 1 (-2.75265) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49065 HOMO: -6.91169 LUMO: 2.02997 factor:1 | 1 (-1.74458) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67528 HOMO: -7.06408 LUMO: 1.41499 factor:1 | 1 (-1.92921) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.37235 HOMO: -6.94162 LUMO: -0.90070 factor:1 | 1 (-2.62628) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79827 HOMO: -7.09401 LUMO: 0.35103 factor:1 | 1 (-2.05220) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.96192 HOMO: -6.78652 LUMO: 0.91974 factor:1 | 1 (-2.21585) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62634 HOMO: -6.32937 LUMO: -1.89119 factor:1 | 1 (-2.88027) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.29045 HOMO: -7.12666 LUMO: -1.06397 factor:1 | 1 (-2.54437) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29679 HOMO: -6.38107 LUMO: -1.43132 factor:1 | 1 (-1.55072) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15442 HOMO: -7.09129 LUMO: 0.08980 factor:1 | 1 (-1.40835) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54760 HOMO: -6.31304 LUMO: -0.57960 factor:1 | 1 (-1.80153) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86203 HOMO: -6.94435 LUMO: -0.74287 factor:1 | 1 (-2.11596) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24738 HOMO: -6.35658 LUMO: -1.53472 factor:1 | 1 (-1.50131) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32392 HOMO: -6.39740 LUMO: -1.48846 factor:1 | 1 (-1.57785) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77182 HOMO: -7.05319 LUMO: -0.33198 factor:1 | 1 (-2.02575) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.18348 HOMO: -6.68040 LUMO: -0.09252 factor:1 | 1 (-2.43741) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40820 HOMO: -6.35930 LUMO: -0.43266 factor:1 | 1 (-1.66213) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40428 HOMO: -6.59604 LUMO: -1.45853 factor:1 | 1 (-1.65821) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99294 HOMO: -6.46270 LUMO: -1.49391 factor:1 | 1 (-2.24687) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67982 HOMO: -7.05863 LUMO: -1.04764 factor:1 | 1 (-1.93375) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64616 HOMO: -7.14027 LUMO: -0.81634 factor:1 | 1 (-1.90009) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.44522 HOMO: -6.80285 LUMO: -0.74287 factor:1 | 1 (-2.69915) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95768 HOMO: -6.53890 LUMO: -1.13471 factor:1 | 1 (-2.21161) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15379 HOMO: -6.49808 LUMO: -1.35513 factor:1 | 1 (-2.40772) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.75464 HOMO: -6.75931 LUMO: -1.49663 factor:1 | 1 (-3.00857) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27652 HOMO: -6.84638 LUMO: -0.77552 factor:1 | 1 (-1.53045) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19372 HOMO: -6.65863 LUMO: -1.34696 factor:1 | 1 (-1.44765) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33394 HOMO: -6.25590 LUMO: -2.36467 factor:1 | 1 (-1.58787) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95798 HOMO: -7.24911 LUMO: 0.33470 factor:1 | 1 (-2.21190) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.36815 HOMO: -6.65863 LUMO: -0.75648 factor:1 | 1 (-3.62208) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42776 HOMO: -6.31576 LUMO: -0.83267 factor:1 | 1 (-1.68169) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25119 HOMO: -6.64774 LUMO: -0.66124 factor:1 | 1 (-1.50512) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28518 HOMO: -6.75387 LUMO: -1.00138 factor:1 | 1 (-1.53910) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.01640 HOMO: -6.52529 LUMO: -0.68301 factor:1 | 1 (-2.27033) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.23863 HOMO: -6.59332 LUMO: -0.68028 factor:1 | 1 (-2.49256) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.19072 HOMO: -5.98650 LUMO: 0.31565 factor:1 | 1 (-2.44464) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84208 HOMO: -6.59876 LUMO: 0.22585 factor:1 | 1 (-2.09601) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.10786 HOMO: -6.72121 LUMO: 0.10340 factor:1 | 1 (-2.36179) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.76637 HOMO: -6.09807 LUMO: 0.20136 factor:1 | 1 (-3.02030) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48925 HOMO: -6.31576 LUMO: 0.06259 factor:1 | 1 (-2.74318) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.29052 HOMO: -6.35658 LUMO: -0.58232 factor:1 | 1 (-3.54445) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.36842 HOMO: -6.34842 LUMO: -0.55783 factor:1 | 1 (-3.62235) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.34585 HOMO: -6.47359 LUMO: -0.57144 factor:1 | 1 (-2.59978) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.47173 HOMO: -6.42189 LUMO: -0.09796 factor:1 | 1 (-2.72566) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.23405 HOMO: -6.35658 LUMO: -0.31293 factor:1 | 1 (-3.48798) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68615 HOMO: -7.35524 LUMO: 0.10340 factor:1 | 1 (-2.94008) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.43252 HOMO: -7.10217 LUMO: 0.36463 factor:1 | 1 (-2.68644) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53294 HOMO: -6.43549 LUMO: -0.56872 factor:1 | 1 (-0.78687) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67491 HOMO: -6.50080 LUMO: -0.71294 factor:1 | 1 (-0.92883) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28820 HOMO: -6.59060 LUMO: -0.57960 factor:1 | 1 (-1.54212) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15083 HOMO: -6.78924 LUMO: -0.31565 factor:1 | 1 (-1.40476) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01282 HOMO: -6.35658 LUMO: 0.07891 factor:1 | 1 (-1.26674) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38632 HOMO: -6.74026 LUMO: -0.87621 factor:1 | 1 (-1.64025) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08855 HOMO: -6.54434 LUMO: 0.81906 factor:1 | 1 (-1.34247) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85514 HOMO: -6.66135 LUMO: 1.40955 factor:1 | 1 (-2.10907) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.39627 HOMO: -6.73754 LUMO: -2.54971 factor:1 | 1 (-2.65020) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.12578 HOMO: -6.65318 LUMO: 0.69389 factor:1 | 1 (-3.37971) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.22369 HOMO: -6.73482 LUMO: 0.62858 factor:1 | 1 (-0.47761) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50187 HOMO: -6.83550 LUMO: 0.68573 factor:1 | 1 (-0.75580) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09614 HOMO: -6.83278 LUMO: 0.45987 factor:1 | 1 (-1.35007) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.95695 HOMO: -6.78380 LUMO: 0.68301 factor:1 | 1 (-1.21088) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02444 HOMO: -6.90625 LUMO: 1.36601 factor:1 | 1 (-1.27836) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70970 HOMO: -6.82734 LUMO: 1.48302 factor:1 | 1 (-1.96363) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64945 HOMO: -6.44094 LUMO: -0.94424 factor:1 | 1 (-2.90337) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30277 HOMO: -6.91441 LUMO: 0.28844 factor:1 | 1 (-2.55670) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19494 HOMO: -6.49808 LUMO: -0.51157 factor:1 | 1 (-1.44887) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07423 HOMO: -7.09673 LUMO: -0.06259 factor:1 | 1 (-1.32816) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10158 HOMO: -6.77019 LUMO: 0.92247 factor:1 | 1 (-1.35551) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75920 HOMO: -6.75931 LUMO: 1.13744 factor:1 | 1 (-2.01313) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.27972 HOMO: -6.15794 LUMO: 1.12383 factor:1 | 1 (-2.53365) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01487 HOMO: -6.59604 LUMO: 1.19458 factor:1 | 1 (-3.26879) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.67257 HOMO: -7.09401 LUMO: 0.60137 factor:1 | 1 (-2.92650) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.42141 HOMO: -6.34025 LUMO: 0.48164 factor:1 | 1 (-2.67534) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.27858 HOMO: -6.72665 LUMO: -2.47624 factor:1 | 1 (-2.53251) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01620 HOMO: -6.48175 LUMO: 0.58232 factor:1 | 1 (-3.27013) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03652 HOMO: -6.94162 LUMO: 0.28300 factor:1 | 1 (-1.29045) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18444 HOMO: -6.65591 LUMO: 0.57144 factor:1 | 1 (-1.43837) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12079 HOMO: -6.58788 LUMO: -1.03947 factor:1 | 1 (-1.37472) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92200 HOMO: -7.18108 LUMO: 0.37824 factor:1 | 1 (-2.17593) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.09931 HOMO: -6.63958 LUMO: -1.52112 factor:1 | 1 (-2.35324) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.21268 HOMO: -6.12528 LUMO: -0.53606 factor:1 | 1 (-2.46660) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.73628 HOMO: -6.22324 LUMO: -0.87893 factor:1 | 1 (-2.99020) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.11401 HOMO: -6.62053 LUMO: -0.91974 factor:1 | 1 (-2.36793) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77627 HOMO: -6.84366 LUMO: -0.83811 factor:1 | 1 (-1.03020) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.21344 HOMO: -7.26000 LUMO: 0.25851 factor:1 | 1 (-2.46737) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77729 HOMO: -6.49536 LUMO: -0.63403 factor:1 | 1 (-2.03122) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74714 HOMO: -6.45726 LUMO: -0.77825 factor:1 | 1 (-2.00107) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72241 HOMO: -6.74570 LUMO: -0.75103 factor:1 | 1 (-1.97634) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.91586 HOMO: -7.20285 LUMO: 0.10612 factor:1 | 1 (-1.16979) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.91042 HOMO: -6.45182 LUMO: -0.56600 factor:1 | 1 (-1.16435) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66693 HOMO: -6.83278 LUMO: -0.71838 factor:1 | 1 (-0.92086) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81861 HOMO: -7.01510 LUMO: -1.09662 factor:1 | 1 (-1.07254) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88544 HOMO: -6.48719 LUMO: 0.16871 factor:1 | 1 (-1.13937) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65874 HOMO: -7.30898 LUMO: 0.26667 factor:1 | 1 (-0.91267) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.78689 HOMO: -6.68856 LUMO: -0.78641 factor:1 | 1 (-3.04082) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.02337 HOMO: -6.56883 LUMO: -1.00682 factor:1 | 1 (-2.27729) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72783 HOMO: -6.41100 LUMO: -0.48980 factor:1 | 1 (-0.98176) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31249 HOMO: -6.52257 LUMO: -0.59865 factor:1 | 1 (-2.56641) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44501 HOMO: -6.63686 LUMO: -0.56055 factor:1 | 1 (-1.69894) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74467 HOMO: -6.79740 LUMO: -0.75376 factor:1 | 1 (-1.99859) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80464 HOMO: -5.89127 LUMO: 0.22313 factor:1 | 1 (-2.05857) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96939 HOMO: -6.34842 LUMO: 0.11429 factor:1 | 1 (-1.22332) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.93997 HOMO: -6.13617 LUMO: 1.94834 factor:1 | 1 (-1.19390) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99586 HOMO: -6.50080 LUMO: 1.74153 factor:1 | 1 (-1.24979) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06381 HOMO: -6.33481 LUMO: 1.68438 factor:1 | 1 (-1.31774) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88035 HOMO: -6.53073 LUMO: 1.95106 factor:1 | 1 (-1.13428) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13641 HOMO: -6.46270 LUMO: 1.89935 factor:1 | 1 (-1.39034) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00152 HOMO: -5.87222 LUMO: 1.91568 factor:1 | 1 (-1.25545) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51715 HOMO: -6.07630 LUMO: 1.81500 factor:1 | 1 (-1.77108) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62415 HOMO: -6.20964 LUMO: 1.81500 factor:1 | 1 (-1.87808) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48602 HOMO: -6.15522 LUMO: 1.90752 factor:1 | 1 (-1.73995) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90228 HOMO: -6.11984 LUMO: 1.95378 factor:1 | 1 (-1.15621) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03557 HOMO: -6.58516 LUMO: 2.04358 factor:1 | 1 (-1.28949) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01039 HOMO: -7.37156 LUMO: 0.24490 factor:1 | 1 (-1.26432) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13238 HOMO: -6.36474 LUMO: -0.90070 factor:1 | 1 (-1.38631) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02863 HOMO: -6.43549 LUMO: -0.40817 factor:1 | 1 (-1.28255) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89488 HOMO: -7.32258 LUMO: 0.29388 factor:1 | 1 (-1.14881) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39644 HOMO: -6.41372 LUMO: -0.20409 factor:1 | 1 (-1.65037) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65715 HOMO: -7.18381 LUMO: 0.42722 factor:1 | 1 (-1.91108) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52646 HOMO: -6.53890 LUMO: -0.54151 factor:1 | 1 (-1.78039) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.95586 HOMO: -6.61509 LUMO: 0.08708 factor:1 | 1 (-1.20979) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47634 HOMO: -6.78108 LUMO: 2.03541 factor:1 | 1 (-1.73026) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49487 HOMO: -6.50896 LUMO: 1.53472 factor:1 | 1 (-1.74879) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53585 HOMO: -6.65591 LUMO: 1.80411 factor:1 | 1 (-1.78977) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46115 HOMO: -6.64502 LUMO: 1.52112 factor:1 | 1 (-1.71508) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26904 HOMO: -6.72938 LUMO: 1.48030 factor:1 | 1 (-1.52297) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55522 HOMO: -6.16882 LUMO: 1.96466 factor:1 | 1 (-1.80915) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41024 HOMO: -6.22597 LUMO: 1.43132 factor:1 | 1 (-1.66417) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12048 HOMO: -6.57699 LUMO: 2.05718 factor:1 | 1 (-2.37441) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94532 HOMO: -6.52529 LUMO: 1.89663 factor:1 | 1 (-2.19925) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20108 HOMO: -6.30760 LUMO: 1.88031 factor:1 | 1 (-2.45501) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.82190 HOMO: -6.14977 LUMO: 1.92657 factor:1 | 1 (-1.07583) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.40013 HOMO: -6.20964 LUMO: 1.83949 factor:1 | 1 (-2.65406) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72725 HOMO: -6.31848 LUMO: 1.91296 factor:1 | 1 (-1.98118) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88756 HOMO: -5.80691 LUMO: 2.19868 factor:1 | 1 (-1.14149) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.87717 HOMO: -6.00827 LUMO: 2.15514 factor:1 | 1 (-1.13110) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70857 HOMO: -6.51713 LUMO: 2.08711 factor:1 | 1 (-0.96249) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81777 HOMO: -6.32937 LUMO: 2.11705 factor:1 | 1 (-1.07169) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44659 HOMO: -6.26678 LUMO: 1.95922 factor:1 | 1 (-1.70052) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56855 HOMO: -6.43005 LUMO: 2.56603 factor:1 | 1 (-1.82248) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86268 HOMO: -6.41644 LUMO: 2.68304 factor:1 | 1 (-2.11661) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46521 HOMO: -5.97834 LUMO: 2.02997 factor:1 | 1 (-1.71913) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43487 HOMO: -6.14161 LUMO: 1.77690 factor:1 | 1 (-0.68880) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38695 HOMO: -6.21508 LUMO: 1.80411 factor:1 | 1 (-0.64088) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.79505 HOMO: -6.46270 LUMO: 2.34562 factor:1 | 1 (-3.04898) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68200 HOMO: -6.39195 LUMO: -0.75920 factor:1 | 1 (-1.93593) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35855 HOMO: -7.08584 LUMO: -1.14016 factor:1 | 1 (-0.61247) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.27499 HOMO: -6.70216 LUMO: -0.65035 factor:1 | 1 (-2.52892) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51751 HOMO: -6.79468 LUMO: -0.83811 factor:1 | 1 (-1.77143) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39168 HOMO: -6.99877 LUMO: -0.79729 factor:1 | 1 (-1.64561) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98911 HOMO: -7.08040 LUMO: -0.85444 factor:1 | 1 (-2.24303) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.80273 HOMO: -7.39333 LUMO: 0.12789 factor:1 | 1 (-3.05665) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.79709 HOMO: -7.05047 LUMO: 0.13878 factor:1 | 1 (-3.05102) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.67826 HOMO: -6.90897 LUMO: -0.77552 factor:1 | 1 (-2.93219) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89928 HOMO: -7.25456 LUMO: 0.05170 factor:1 | 1 (-2.15321) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51597 HOMO: -6.84638 LUMO: -0.84355 factor:1 | 1 (-2.76990) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58924 HOMO: -6.78108 LUMO: -0.81634 factor:1 | 1 (-0.84317) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.97396 HOMO: -6.74570 LUMO: -0.77280 factor:1 | 1 (-1.22789) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32588 HOMO: -7.28177 LUMO: -1.68438 factor:1 | 1 (-1.57981) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58692 HOMO: -7.22190 LUMO: -1.63540 factor:1 | 1 (-1.84085) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.02170 HOMO: -7.15932 LUMO: -1.57554 factor:1 | 1 (-3.27563) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.76858 HOMO: -6.57971 LUMO: -0.93063 factor:1 | 1 (-3.02250) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53179 HOMO: -6.88176 LUMO: 0.58232 factor:1 | 1 (-1.78572) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50638 HOMO: -6.85727 LUMO: 0.51430 factor:1 | 1 (-1.76030) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69343 HOMO: -6.83550 LUMO: 0.87893 factor:1 | 1 (-1.94736) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.95043 HOMO: -7.06680 LUMO: 0.87621 factor:1 | 1 (-3.20436) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.11035 HOMO: -6.52257 LUMO: 0.81362 factor:1 | 1 (-3.36428) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.83671 HOMO: -6.95523 LUMO: 1.17009 factor:1 | 1 (-3.09064) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.94077 HOMO: -7.21374 LUMO: 0.97145 factor:1 | 1 (-3.19470) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.94918 HOMO: -6.81373 LUMO: -1.54561 factor:1 | 1 (-3.20311) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65637 HOMO: -6.86543 LUMO: -1.52656 factor:1 | 1 (-1.91029) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68208 HOMO: -6.90081 LUMO: -0.78097 factor:1 | 1 (-1.93601) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60724 HOMO: -6.64502 LUMO: -0.82723 factor:1 | 1 (-2.86117) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62332 HOMO: -6.65591 LUMO: -0.82178 factor:1 | 1 (-2.87725) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08071 HOMO: -6.79468 LUMO: -1.46397 factor:1 | 1 (-1.33464) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35739 HOMO: -7.25728 LUMO: 0.73743 factor:1 | 1 (-1.61132) | 1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03836 HOMO: -7.00149 LUMO: 1.30070 factor:1 | 1 (-2.29229) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94184 HOMO: -7.07768 LUMO: 0.78097 factor:1 | 1 (-2.19577) | 1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15096 HOMO: -6.86271 LUMO: 0.86260 factor:1 | 1 (-2.40489) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74510 HOMO: -6.94707 LUMO: 0.39729 factor:1 | 1 (-1.99903) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78445 HOMO: -6.79740 LUMO: 0.67484 factor:1 | 1 (-2.03838) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99820 HOMO: -6.91986 LUMO: -1.14288 factor:1 | 1 (-2.25212) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00549 HOMO: -6.31576 LUMO: 1.01771 factor:1 | 1 (-2.25942) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48705 HOMO: -6.81645 LUMO: 0.81362 factor:1 | 1 (-2.74098) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.47769 HOMO: -6.92258 LUMO: -0.99594 factor:1 | 1 (-2.73161) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.39281 HOMO: -6.81373 LUMO: 0.61770 factor:1 | 1 (-2.64674) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.74270 HOMO: -7.18653 LUMO: 1.19186 factor:1 | 1 (-2.99663) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74777 HOMO: -7.00693 LUMO: 0.45715 factor:1 | 1 (-2.00170) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63441 HOMO: -7.11306 LUMO: 0.53334 factor:1 | 1 (-1.88833) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01576 HOMO: -6.63414 LUMO: -1.64357 factor:1 | 1 (-3.26969) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.84836 HOMO: -6.22052 LUMO: -0.74015 factor:1 | 1 (-3.10229) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.86575 HOMO: -6.81101 LUMO: -0.50069 factor:1 | 1 (-3.11968) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.87905 HOMO: -6.71849 LUMO: -0.51974 factor:1 | 1 (-1.13297) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24289 HOMO: -6.72121 LUMO: -1.77690 factor:1 | 1 (-1.49682) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87612 HOMO: -6.94162 LUMO: -1.78779 factor:1 | 1 (-2.13005) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99022 HOMO: -6.91169 LUMO: 0.88981 factor:1 | 1 (-2.24415) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73756 HOMO: -6.97428 LUMO: 0.70750 factor:1 | 1 (-1.99149) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57568 HOMO: -6.74842 LUMO: 1.15921 factor:1 | 1 (-1.82961) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47002 HOMO: -7.25183 LUMO: -0.99594 factor:1 | 1 (-1.72395) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.27714 HOMO: -6.43821 LUMO: -1.00410 factor:1 | 1 (-2.53107) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.25888 HOMO: -6.52257 LUMO: -0.68573 factor:1 | 1 (-2.51281) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72705 HOMO: -6.60148 LUMO: -0.52518 factor:1 | 1 (-2.98098) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.92795 HOMO: -6.07086 LUMO: -1.39594 factor:1 | 1 (-3.18188) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82840 HOMO: -6.78108 LUMO: -1.54833 factor:1 | 1 (-2.08232) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66945 HOMO: -6.73482 LUMO: -1.01498 factor:1 | 1 (-1.92338) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85944 HOMO: -6.85183 LUMO: 1.06669 factor:1 | 1 (-2.11337) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.98442 HOMO: -6.98516 LUMO: 1.43948 factor:1 | 1 (-3.23835) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69879 HOMO: -6.94162 LUMO: 0.79185 factor:1 | 1 (-1.95272) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62039 HOMO: -6.67495 LUMO: -1.06669 factor:1 | 1 (-1.87432) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.70792 HOMO: -6.88720 LUMO: -1.00682 factor:1 | 1 (-2.96185) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76717 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-2.02110) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72069 HOMO: -6.51713 LUMO: -0.89798 factor:1 | 1 (-1.97462) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54665 HOMO: -6.63141 LUMO: -0.91430 factor:1 | 1 (-1.80058) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61136 HOMO: -6.63414 LUMO: 0.04354 factor:1 | 1 (-1.86529) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79669 HOMO: -6.65046 LUMO: -0.73743 factor:1 | 1 (-2.05062) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73795 HOMO: -6.73754 LUMO: -0.71838 factor:1 | 1 (-1.99187) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77229 HOMO: -6.65863 LUMO: -0.60137 factor:1 | 1 (-2.02621) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42817 HOMO: -6.61509 LUMO: -0.47892 factor:1 | 1 (-1.68210) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99520 HOMO: -6.82189 LUMO: -0.64763 factor:1 | 1 (-2.24913) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87495 HOMO: -6.56883 LUMO: -0.51974 factor:1 | 1 (-2.12888) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.27042 HOMO: -6.97428 LUMO: -0.95512 factor:1 | 1 (-2.52435) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51178 HOMO: -6.70489 LUMO: -0.04082 factor:1 | 1 (-2.76571) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65054 HOMO: -6.74026 LUMO: 0.02177 factor:1 | 1 (-1.90447) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57691 HOMO: -6.50080 LUMO: -0.89525 factor:1 | 1 (-1.83084) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58088 HOMO: -6.46815 LUMO: -0.61226 factor:1 | 1 (-1.83481) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.73640 HOMO: -6.57971 LUMO: -0.64219 factor:1 | 1 (-3.99033) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.81728 HOMO: -7.17836 LUMO: 0.37280 factor:1 | 1 (-3.07121) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78720 HOMO: -6.67223 LUMO: 0.12245 factor:1 | 1 (-2.04113) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55862 HOMO: -6.55250 LUMO: 0.22858 factor:1 | 1 (-1.81255) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46303 HOMO: -6.97156 LUMO: -1.12927 factor:1 | 1 (-1.71696) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60066 HOMO: -6.78924 LUMO: -0.84900 factor:1 | 1 (-2.85458) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50903 HOMO: -6.65046 LUMO: -0.65307 factor:1 | 1 (-2.76296) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.21602 HOMO: -7.41782 LUMO: 0.08980 factor:1 | 1 (-2.46995) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.29377 HOMO: -6.56339 LUMO: -0.68573 factor:1 | 1 (-2.54769) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.76901 HOMO: -6.31032 LUMO: -0.31837 factor:1 | 1 (-3.02294) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.79900 HOMO: -6.72938 LUMO: -0.45987 factor:1 | 1 (-3.05293) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.78296 HOMO: -6.59876 LUMO: -1.03131 factor:1 | 1 (-4.03689) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64841 HOMO: -7.29265 LUMO: 0.29660 factor:1 | 1 (-2.90234) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68338 HOMO: -6.42189 LUMO: -0.51157 factor:1 | 1 (-2.93731) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.97693 HOMO: -6.27767 LUMO: -0.52790 factor:1 | 1 (-3.23086) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88734 HOMO: -6.41644 LUMO: -0.44627 factor:1 | 1 (-2.14126) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.35450 HOMO: -6.23413 LUMO: -0.52790 factor:1 | 1 (-2.60843) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.79824 HOMO: -6.63414 LUMO: -0.44082 factor:1 | 1 (-3.05217) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85439 HOMO: -7.03142 LUMO: 0.47076 factor:1 | 1 (-1.10832) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86987 HOMO: -6.62053 LUMO: -0.14422 factor:1 | 1 (-2.12379) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47465 HOMO: -6.22324 LUMO: 1.96194 factor:1 | 1 (-1.72858) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38893 HOMO: -6.17971 LUMO: 1.71704 factor:1 | 1 (-1.64286) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71141 HOMO: -6.70761 LUMO: 1.68711 factor:1 | 1 (-1.96534) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.29782 HOMO: -6.52801 LUMO: 1.56193 factor:1 | 1 (-2.55175) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.74351 HOMO: -6.55794 LUMO: 1.52384 factor:1 | 1 (-2.99744) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60503 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-0.85895) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76742 HOMO: -6.65863 LUMO: 1.83133 factor:1 | 1 (-2.02134) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34177 HOMO: -6.46270 LUMO: 1.90208 factor:1 | 1 (-1.59570) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26813 HOMO: -6.41917 LUMO: 2.03269 factor:1 | 1 (-2.52206) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.04260 HOMO: -6.48992 LUMO: 1.87486 factor:1 | 1 (-3.29652) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68822 HOMO: -6.51985 LUMO: 1.69527 factor:1 | 1 (-2.94215) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60485 HOMO: -6.36202 LUMO: 2.05718 factor:1 | 1 (-1.85878) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39549 HOMO: -5.96474 LUMO: 1.88575 factor:1 | 1 (-1.64942) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.39271 HOMO: -6.56339 LUMO: 2.04630 factor:1 | 1 (-2.64663) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.60152 HOMO: -6.43277 LUMO: 1.98371 factor:1 | 1 (-3.85545) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.03590 HOMO: -6.53345 LUMO: 2.06262 factor:1 | 1 (-3.28983) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.73949 HOMO: -5.81779 LUMO: 2.11432 factor:1 | 1 (-2.99342) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.61262 HOMO: -5.91848 LUMO: 1.86942 factor:1 | 1 (-3.86655) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43544 HOMO: -6.48447 LUMO: 1.70343 factor:1 | 1 (-1.68936) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43416 HOMO: -6.29671 LUMO: -0.89525 factor:1 | 1 (-1.68809) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.42163 HOMO: -6.63414 LUMO: -0.76192 factor:1 | 1 (-2.67556) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53721 HOMO: -6.56883 LUMO: -0.86260 factor:1 | 1 (-1.79114) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34357 HOMO: -6.93074 LUMO: -0.27483 factor:1 | 1 (-1.59750) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78440 HOMO: -6.85999 LUMO: -0.01905 factor:1 | 1 (-2.03832) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67321 HOMO: -6.26406 LUMO: 0.21769 factor:1 | 1 (-1.92714) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41964 HOMO: -6.62325 LUMO: 0.31293 factor:1 | 1 (-0.67356) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34244 HOMO: -6.59604 LUMO: 0.19592 factor:1 | 1 (-0.59636) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47749 HOMO: -6.43277 LUMO: -0.27756 factor:1 | 1 (-0.73141) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55596 HOMO: -6.54978 LUMO: -0.46531 factor:1 | 1 (-0.80989) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42698 HOMO: -6.65046 LUMO: -0.15783 factor:1 | 1 (-0.68091) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56195 HOMO: -7.28721 LUMO: 0.23946 factor:1 | 1 (-0.81588) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70699 HOMO: -6.71849 LUMO: -0.56600 factor:1 | 1 (-0.96092) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43716 HOMO: -6.85183 LUMO: -0.84355 factor:1 | 1 (-0.69109) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62024 HOMO: -6.53345 LUMO: -0.84627 factor:1 | 1 (-0.87417) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33904 HOMO: -6.60148 LUMO: -0.63130 factor:1 | 1 (-0.59296) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63880 HOMO: -6.36202 LUMO: -0.60137 factor:1 | 1 (-0.89272) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36739 HOMO: -6.28855 LUMO: -0.52790 factor:1 | 1 (-0.62132) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35664 HOMO: -7.07224 LUMO: 0.41906 factor:1 | 1 (-0.61057) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58418 HOMO: -6.36202 LUMO: -0.24218 factor:1 | 1 (-0.83811) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53659 HOMO: -6.43549 LUMO: 0.14150 factor:1 | 1 (-0.79052) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62002 HOMO: -6.76747 LUMO: -0.40545 factor:1 | 1 (-0.87395) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49602 HOMO: -6.15249 LUMO: -0.51157 factor:1 | 1 (-0.74995) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58473 HOMO: -6.33753 LUMO: -0.02993 factor:1 | 1 (-0.83865) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38916 HOMO: -6.49808 LUMO: -0.83811 factor:1 | 1 (-0.64309) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42853 HOMO: -6.64502 LUMO: -0.46259 factor:1 | 1 (-0.68246) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59458 HOMO: -6.34570 LUMO: 0.22041 factor:1 | 1 (-0.84851) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10642 HOMO: -6.63414 LUMO: -0.13606 factor:1 | 1 (-1.36035) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21894 HOMO: -6.59604 LUMO: -0.79729 factor:1 | 1 (-1.47287) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10090 HOMO: -7.09401 LUMO: 0.31837 factor:1 | 1 (-1.35483) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00433 HOMO: -6.48719 LUMO: -0.31021 factor:1 | 1 (-1.25825) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52228 HOMO: -7.11306 LUMO: 0.39729 factor:1 | 1 (-0.77620) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52810 HOMO: -6.95251 LUMO: 0.41089 factor:1 | 1 (-0.78203) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50668 HOMO: -6.61509 LUMO: -0.41906 factor:1 | 1 (-0.76061) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38070 HOMO: -6.25318 LUMO: -0.47348 factor:1 | 1 (-0.63462) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.69578 HOMO: -6.77019 LUMO: -0.10340 factor:1 | 1 (-0.94970) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75922 HOMO: -6.54706 LUMO: -0.46259 factor:1 | 1 (-2.01315) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77558 HOMO: -6.34297 LUMO: -0.50341 factor:1 | 1 (-2.02951) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43416 HOMO: -6.20692 LUMO: -0.51974 factor:1 | 1 (-1.68809) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.69012 HOMO: -7.03686 LUMO: 0.46804 factor:1 | 1 (-0.94404) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.45999 HOMO: -6.47087 LUMO: 0.22585 factor:1 | 1 (-0.71392) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76682 HOMO: -6.41917 LUMO: 0.19320 factor:1 | 1 (-2.02074) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26639 HOMO: -6.61237 LUMO: -0.04354 factor:1 | 1 (-2.52032) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79923 HOMO: -6.56339 LUMO: 0.36735 factor:1 | 1 (-2.05315) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.57596 HOMO: -6.54978 LUMO: 1.12655 factor:1 | 1 (-0.82989) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39977 HOMO: -6.43277 LUMO: 1.17553 factor:1 | 1 (-0.65370) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97101 HOMO: -6.29944 LUMO: 1.40955 factor:1 | 1 (-2.22494) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55367 HOMO: -6.74842 LUMO: 0.74015 factor:1 | 1 (-1.80760) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19203 HOMO: -6.15522 LUMO: 1.94289 factor:1 | 1 (-1.44596) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47217 HOMO: -6.20147 LUMO: 1.40139 factor:1 | 1 (-1.72610) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93327 HOMO: -6.41100 LUMO: 1.40139 factor:1 | 1 (-2.18720) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08479 HOMO: -6.74570 LUMO: 1.80956 factor:1 | 1 (-1.33872) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42156 HOMO: -6.60148 LUMO: -1.04764 factor:1 | 1 (-1.67549) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73141 HOMO: -6.82734 LUMO: -0.83267 factor:1 | 1 (-1.98534) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66227 HOMO: -7.01782 LUMO: -0.32382 factor:1 | 1 (-1.91620) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77251 HOMO: -6.54434 LUMO: 0.11157 factor:1 | 1 (-1.02644) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79357 HOMO: -6.53617 LUMO: 0.32926 factor:1 | 1 (-1.04750) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.80255 HOMO: -6.62597 LUMO: -0.60137 factor:1 | 1 (-1.05648) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.80772 HOMO: -6.60965 LUMO: -0.75376 factor:1 | 1 (-1.06165) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64862 HOMO: -6.29399 LUMO: 0.06803 factor:1 | 1 (-0.90255) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58701 HOMO: -6.60692 LUMO: -0.47076 factor:1 | 1 (-0.84094) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99351 HOMO: -7.33891 LUMO: 0.39184 factor:1 | 1 (-2.24744) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64345 HOMO: -6.60692 LUMO: 1.46125 factor:1 | 1 (-0.89738) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12250 HOMO: -6.21780 LUMO: 2.09256 factor:1 | 1 (-2.37642) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66812 HOMO: -6.28311 LUMO: 1.80411 factor:1 | 1 (-1.92205) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70837 HOMO: -6.51168 LUMO: 1.84765 factor:1 | 1 (-1.96229) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72290 HOMO: -6.66951 LUMO: 2.01636 factor:1 | 1 (-1.97683) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26704 HOMO: -6.75387 LUMO: 1.73881 factor:1 | 1 (-2.52097) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84968 HOMO: -6.77291 LUMO: 1.89935 factor:1 | 1 (-2.10360) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85664 HOMO: -6.36474 LUMO: 1.61091 factor:1 | 1 (-2.11057) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37368 HOMO: -6.60420 LUMO: 1.40955 factor:1 | 1 (-0.62760) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30183 HOMO: -6.81645 LUMO: 1.59731 factor:1 | 1 (-1.55576) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48804 HOMO: -5.90215 LUMO: 2.12249 factor:1 | 1 (-1.74196) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58243 HOMO: -6.26950 LUMO: 1.62996 factor:1 | 1 (-1.83636) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63204 HOMO: -6.41100 LUMO: 1.80684 factor:1 | 1 (-1.88597) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70747 HOMO: -6.64230 LUMO: 2.23405 factor:1 | 1 (-1.96140) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68679 HOMO: -6.66951 LUMO: 2.21501 factor:1 | 1 (-1.94072) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37217 HOMO: -6.90897 LUMO: 2.00004 factor:1 | 1 (-1.62610) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90489 HOMO: -6.61781 LUMO: 1.42043 factor:1 | 1 (-2.15882) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44545 HOMO: -6.56611 LUMO: 1.60003 factor:1 | 1 (-1.69938) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63572 HOMO: -6.70489 LUMO: 1.78779 factor:1 | 1 (-0.88965) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.69776 HOMO: -6.46815 LUMO: 1.59459 factor:1 | 1 (-0.95169) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60943 HOMO: -6.31304 LUMO: 1.36873 factor:1 | 1 (-0.86336) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.69825 HOMO: -6.22597 LUMO: 1.54833 factor:1 | 1 (-0.95218) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.68810 HOMO: -5.63004 LUMO: 1.96466 factor:1 | 1 (-0.94203) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63520 HOMO: -7.02598 LUMO: 1.79323 factor:1 | 1 (-0.88913) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46067 HOMO: -6.78924 LUMO: 2.10888 factor:1 | 1 (-0.71460) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.03378 HOMO: -6.13345 LUMO: 2.07351 factor:1 | 1 (-0.28771) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81314 HOMO: -6.46270 LUMO: -0.37552 factor:1 | 1 (-1.06707) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23146 HOMO: -6.51985 LUMO: -0.49525 factor:1 | 1 (-1.48539) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72530 HOMO: -6.60965 LUMO: 1.90480 factor:1 | 1 (-0.97923) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66135 HOMO: -6.51168 LUMO: 1.92112 factor:1 | 1 (-1.91527) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.33690 HOMO: -6.71305 LUMO: 1.91024 factor:1 | 1 (-2.59082) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85471 HOMO: -6.86815 LUMO: 2.02997 factor:1 | 1 (-2.10864) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.56591 HOMO: -6.69944 LUMO: 1.95106 factor:1 | -1 (0.18017) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.72966 HOMO: -6.45182 LUMO: 1.66806 factor:1 | -1 (0.01641) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.81116 HOMO: -6.44638 LUMO: 2.16058 factor:1 | 1 (-0.06509) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72782 HOMO: -6.65591 LUMO: 1.95106 factor:1 | 1 (-1.98175) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20824 HOMO: -6.35114 LUMO: 1.42316 factor:1 | 1 (-2.46217) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70322 HOMO: -6.48719 LUMO: 1.59187 factor:1 | 1 (-1.95715) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88276 HOMO: -7.05591 LUMO: 1.61908 factor:1 | 1 (-2.13669) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82004 HOMO: -6.92258 LUMO: 1.87214 factor:1 | 1 (-2.07397) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17386 HOMO: -5.85861 LUMO: 2.11705 factor:1 | 1 (-0.42779) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.05703 HOMO: -6.27767 LUMO: 1.75513 factor:1 | -1 (0.68905) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.44315 HOMO: -6.16882 LUMO: 1.73881 factor:1 | -1 (0.30292) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.44677 HOMO: -6.62053 LUMO: 1.39594 factor:1 | -1 (0.29930) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.02102 HOMO: -5.46405 LUMO: 1.68166 factor:1 | 1 (-0.27494) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.18349 HOMO: -6.39740 LUMO: 1.68711 factor:1 | 1 (-0.43742) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.23961 HOMO: -6.99333 LUMO: 2.08439 factor:1 | 1 (-3.49353) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62603 HOMO: -6.16882 LUMO: 1.71976 factor:1 | 1 (-0.87996) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69318 HOMO: -7.19741 LUMO: 2.24766 factor:1 | 1 (-1.94711) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.00396 HOMO: -6.77291 LUMO: 2.17691 factor:1 | 1 (-3.25788) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66842 HOMO: -6.29944 LUMO: 2.16603 factor:1 | 1 (-1.92235) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.75406 HOMO: -6.10079 LUMO: 1.83949 factor:1 | 1 (-4.00799) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.32900 HOMO: -6.63686 LUMO: 2.05990 factor:1 | 1 (-3.58292) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58377 HOMO: -6.91713 LUMO: 1.87486 factor:1 | 1 (-0.83770) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.05144 HOMO: -6.63958 LUMO: 1.79323 factor:1 | 1 (-0.30537) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.23066 HOMO: -6.61781 LUMO: 1.70071 factor:1 | -1 (0.51541) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.48786 HOMO: -6.20420 LUMO: 1.82861 factor:1 | -1 (0.25821) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.16174 HOMO: -6.47903 LUMO: -2.16875 factor:1 | 1 (-2.41566) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72733 HOMO: -6.53073 LUMO: 2.18235 factor:1 | 1 (-1.98126) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52611 HOMO: -7.01782 LUMO: 1.72520 factor:1 | 1 (-0.78004) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.95477 HOMO: -6.66135 LUMO: -0.75648 factor:1 | 1 (-1.20870) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51066 HOMO: -7.56749 LUMO: 0.22585 factor:1 | 1 (-0.76459) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46888 HOMO: -6.45182 LUMO: -0.71294 factor:1 | 1 (-1.72281) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78075 HOMO: -6.31032 LUMO: -0.34286 factor:1 | 1 (-2.03468) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53623 HOMO: -6.41917 LUMO: 2.04085 factor:1 | 1 (-1.79016) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.91179 HOMO: -6.61781 LUMO: 1.98915 factor:1 | 1 (-3.16572) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.69172 HOMO: -5.86405 LUMO: 1.57282 factor:1 | 1 (-3.94565) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.06292 HOMO: -6.44094 LUMO: 1.80956 factor:1 | 1 (-3.31685) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66840 HOMO: -6.59060 LUMO: 2.08167 factor:1 | 1 (-0.92233) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66339 HOMO: -6.20147 LUMO: 1.69799 factor:1 | 1 (-0.91732) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64086 HOMO: -6.50352 LUMO: -0.41361 factor:1 | 1 (-0.89479) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53645 HOMO: -6.10896 LUMO: -0.55783 factor:1 | 1 (-0.79038) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.14437 HOMO: -6.74842 LUMO: -0.56872 factor:1 | 1 (-3.39829) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37604 HOMO: -6.59060 LUMO: -0.22041 factor:1 | 1 (-0.62997) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51188 HOMO: -6.22052 LUMO: -0.60137 factor:1 | 1 (-0.76581) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.04089 HOMO: -6.65863 LUMO: 0.07891 factor:1 | 1 (-2.29482) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64753 HOMO: -6.57427 LUMO: 1.71160 factor:1 | 1 (-0.90146) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73158 HOMO: -5.84773 LUMO: 1.99459 factor:1 | 1 (-1.98551) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.44324 HOMO: -6.02188 LUMO: 1.91296 factor:1 | 1 (-2.69717) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67490 HOMO: -6.17698 LUMO: 2.00004 factor:1 | 1 (-1.92882) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14384 HOMO: -6.02732 LUMO: 1.90752 factor:1 | 1 (-1.39777) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42262 HOMO: -6.68584 LUMO: -0.50885 factor:1 | 1 (-1.67655) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48701 HOMO: -6.61781 LUMO: -0.73471 factor:1 | 1 (-0.74094) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55126 HOMO: -6.66407 LUMO: -0.79729 factor:1 | 1 (-0.80518) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37165 HOMO: -6.56339 LUMO: 0.23130 factor:1 | 1 (-1.62558) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72203 HOMO: -6.76747 LUMO: 0.08980 factor:1 | 1 (-1.97595) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.18087 HOMO: -6.70489 LUMO: -0.53334 factor:1 | 1 (-2.43479) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36850 HOMO: -7.28993 LUMO: 0.10885 factor:1 | 1 (-1.62242) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68314 HOMO: -6.22052 LUMO: 0.51974 factor:1 | 1 (-1.93707) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30628 HOMO: -6.81645 LUMO: 0.25307 factor:1 | 1 (-2.56021) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13920 HOMO: -6.80285 LUMO: 0.02721 factor:1 | 1 (-2.39313) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.67785 HOMO: -6.51441 LUMO: 0.08163 factor:1 | 1 (-2.93178) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39105 HOMO: -6.73482 LUMO: -0.77008 factor:1 | 1 (-1.64498) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39756 HOMO: -6.29127 LUMO: -0.44355 factor:1 | 1 (-1.65149) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.41616 HOMO: -6.72938 LUMO: -0.64763 factor:1 | 1 (-2.67009) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53341 HOMO: -6.49264 LUMO: -0.74559 factor:1 | 1 (-0.78733) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84876 HOMO: -6.67223 LUMO: -0.55239 factor:1 | 1 (-1.10269) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10626 HOMO: -6.33481 LUMO: 0.33198 factor:1 | 1 (-1.36019) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99371 HOMO: -6.76475 LUMO: -0.25307 factor:1 | 1 (-1.24764) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34624 HOMO: -6.65318 LUMO: 0.03810 factor:1 | 1 (-1.60017) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46088 HOMO: -6.09263 LUMO: 0.21497 factor:1 | 1 (-1.71481) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.37183 HOMO: -6.32120 LUMO: -0.85444 factor:1 | 1 (-2.62576) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.71853 HOMO: -6.57155 LUMO: -0.67484 factor:1 | 1 (-2.97246) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.23582 HOMO: -6.53345 LUMO: -0.78913 factor:1 | 1 (-0.48975) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66508 HOMO: -7.07768 LUMO: 0.28844 factor:1 | 1 (-0.91901) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00414 HOMO: -6.75114 LUMO: 0.18776 factor:1 | 1 (-1.25806) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28373 HOMO: -6.77019 LUMO: -0.12245 factor:1 | 1 (-1.53766) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.66950 HOMO: -6.43549 LUMO: 0.16327 factor:1 | 1 (-2.92343) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30911 HOMO: -6.69400 LUMO: -0.16327 factor:1 | 1 (-2.56304) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22466 HOMO: -6.38651 LUMO: -0.61770 factor:1 | 1 (-1.47859) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.05497 HOMO: -6.34297 LUMO: -0.33198 factor:1 | 1 (-1.30889) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32577 HOMO: -7.51578 LUMO: 0.02177 factor:1 | 1 (-1.57970) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57121 HOMO: -6.47359 LUMO: -0.22585 factor:1 | 1 (-2.82514) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68207 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-2.93600) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.40120 HOMO: -6.75659 LUMO: -0.57688 factor:1 | 1 (-2.65512) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56727 HOMO: -6.73754 LUMO: -0.61226 factor:1 | 1 (-2.82119) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33960 HOMO: -7.37429 LUMO: 0.31293 factor:1 | 1 (-1.59353) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51680 HOMO: -6.23413 LUMO: -0.90886 factor:1 | 1 (-1.77073) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59088 HOMO: -6.51985 LUMO: -0.68028 factor:1 | 1 (-0.84480) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63028 HOMO: -6.52257 LUMO: -0.77280 factor:1 | 1 (-0.88421) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52802 HOMO: -7.29537 LUMO: 0.31837 factor:1 | 1 (-0.78195) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.45730 HOMO: -6.08447 LUMO: 0.25851 factor:1 | 1 (-0.71122) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48143 HOMO: -6.20964 LUMO: 0.13606 factor:1 | 1 (-0.73536) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.30576 HOMO: -6.49808 LUMO: -0.14150 factor:1 | 1 (-0.55968) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75873 HOMO: -7.10761 LUMO: 0.28028 factor:1 | 1 (-2.01266) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.53453 HOMO: -6.60965 LUMO: -0.62858 factor:1 | 1 (-2.78846) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44818 HOMO: -6.40012 LUMO: -0.26939 factor:1 | 1 (-0.70211) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33867 HOMO: -6.65318 LUMO: -0.73199 factor:1 | 1 (-1.59260) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53800 HOMO: -6.51441 LUMO: -0.44899 factor:1 | 1 (-1.79192) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26741 HOMO: -6.28583 LUMO: -0.48708 factor:1 | 1 (-1.52133) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48851 HOMO: -6.96884 LUMO: 0.19864 factor:1 | 1 (-0.74244) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48024 HOMO: -6.89809 LUMO: 0.34558 factor:1 | 1 (-0.73416) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21422 HOMO: -6.67495 LUMO: -0.15510 factor:1 | 1 (-0.46814) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48881 HOMO: -7.34980 LUMO: 0.19864 factor:1 | 1 (-0.74273) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39384 HOMO: -6.71305 LUMO: -0.81634 factor:1 | 1 (-0.64777) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.09060 HOMO: -6.39468 LUMO: -0.47076 factor:1 | 1 (-0.34452) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42127 HOMO: -6.31304 LUMO: 1.39594 factor:1 | 1 (-0.67520) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.26622 HOMO: -6.57155 LUMO: 1.55105 factor:1 | 1 (-0.52015) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34763 HOMO: -6.68312 LUMO: 1.69255 factor:1 | 1 (-1.60155) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33508 HOMO: -6.61509 LUMO: 1.73881 factor:1 | 1 (-1.58901) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.01112 HOMO: -6.17971 LUMO: 1.90208 factor:1 | 1 (-2.26505) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86472 HOMO: -6.53073 LUMO: 1.73337 factor:1 | 1 (-2.11865) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42028 HOMO: -5.91303 LUMO: 1.90480 factor:1 | 1 (-1.67421) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.06156 HOMO: -6.42733 LUMO: 1.80139 factor:1 | 1 (-0.31549) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39917 HOMO: -6.78924 LUMO: 2.31569 factor:1 | 1 (-0.65310) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12909 HOMO: -6.04093 LUMO: 1.91568 factor:1 | 1 (-1.38302) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.06043 HOMO: -6.90081 LUMO: 2.36739 factor:1 | 1 (-2.31436) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41734 HOMO: -6.60965 LUMO: 2.18507 factor:1 | 1 (-1.67127) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74290 HOMO: -6.75387 LUMO: 2.48712 factor:1 | 1 (-1.99683) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.43456 HOMO: -6.56883 LUMO: 1.71432 factor:1 | 1 (-2.68848) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34357 HOMO: -6.41644 LUMO: 1.72792 factor:1 | 1 (-1.59750) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.16779 HOMO: -6.92530 LUMO: 2.54426 factor:1 | 1 (-0.42172) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34619 HOMO: -6.41644 LUMO: 2.70209 factor:1 | 1 (-0.60012) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.11568 HOMO: -6.29671 LUMO: 2.14698 factor:1 | 1 (-0.36961) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20760 HOMO: -6.29127 LUMO: 1.87486 factor:1 | 1 (-1.46152) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92527 HOMO: -6.75931 LUMO: 2.78917 factor:1 | 1 (-2.17920) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40559 HOMO: -6.40828 LUMO: 1.86942 factor:1 | 1 (-1.65951) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09655 HOMO: -6.45726 LUMO: 1.97010 factor:1 | 1 (-1.35047) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25375 HOMO: -6.43277 LUMO: 1.22723 factor:1 | 1 (-1.50767) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50757 HOMO: -6.63414 LUMO: 1.62452 factor:1 | 1 (-1.76150) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86880 HOMO: -6.54162 LUMO: 2.16058 factor:1 | 1 (-2.12273) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15584 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-1.40977) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09780 HOMO: -6.20964 LUMO: 1.84221 factor:1 | 1 (-1.35173) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34232 HOMO: -6.58516 LUMO: 1.69799 factor:1 | 1 (-1.59625) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83490 HOMO: -6.44094 LUMO: 2.05446 factor:1 | 1 (-2.08883) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.61764 HOMO: -6.61509 LUMO: 2.16058 factor:1 | 1 (-2.87156) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88540 HOMO: -6.65591 LUMO: 1.69527 factor:1 | 1 (-2.13933) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.76642 HOMO: -5.55112 LUMO: 1.80411 factor:1 | 1 (-4.02035) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.69510 HOMO: -6.68312 LUMO: 2.38100 factor:1 | 1 (-0.94902) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.40930 HOMO: -6.51168 LUMO: 2.14698 factor:1 | 1 (-2.66323) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.74324 HOMO: -6.04637 LUMO: 1.48302 factor:1 | 1 (-2.99717) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87983 HOMO: -6.81645 LUMO: -0.74287 factor:1 | 1 (-2.13375) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48623 HOMO: -6.96884 LUMO: -0.97961 factor:1 | 1 (-2.74016) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94897 HOMO: -6.45998 LUMO: 0.09796 factor:1 | 1 (-2.20290) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66152 HOMO: -6.44638 LUMO: 0.09524 factor:1 | 1 (-0.91545) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.18390 HOMO: -6.16338 LUMO: -0.54151 factor:1 | 1 (-0.43783) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70059 HOMO: -6.35930 LUMO: -0.47892 factor:1 | 1 (-0.95452) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35724 HOMO: -6.65318 LUMO: -0.00272 factor:1 | 1 (-0.61117) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78537 HOMO: -6.50080 LUMO: 0.14694 factor:1 | 1 (-2.03930) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00108 HOMO: -6.60420 LUMO: 0.94968 factor:1 | 1 (-2.25501) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.12885 HOMO: -6.60148 LUMO: -0.77552 factor:1 | 1 (-0.38278) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.72841 HOMO: -6.81645 LUMO: -1.05580 factor:1 | -1 (0.01766) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.49263 HOMO: -6.57971 LUMO: -0.82178 factor:1 | -1 (0.25345) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.03386 HOMO: -6.09263 LUMO: -0.45171 factor:1 | 1 (-0.28779) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.63445 HOMO: -6.74298 LUMO: -0.61770 factor:1 | -1 (0.11162) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53792 HOMO: -6.72393 LUMO: 1.21091 factor:1 | 1 (-0.79185) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50791 HOMO: -6.30488 LUMO: 1.70071 factor:1 | 1 (-0.76184) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.55222 HOMO: -6.38107 LUMO: 1.55649 factor:1 | -1 (0.19385) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.56403 HOMO: -6.17154 LUMO: 1.46669 factor:1 | -1 (0.18204) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.68534 HOMO: -6.86543 LUMO: 1.98643 factor:1 | -1 (0.06074) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15723 HOMO: -6.69944 LUMO: 1.65173 factor:1 | 1 (-1.41116) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07940 HOMO: -6.77836 LUMO: 2.16331 factor:1 | 1 (-1.33333) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73420 HOMO: -6.42189 LUMO: 2.36467 factor:1 | 1 (-0.98813) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81057 HOMO: -7.00965 LUMO: 2.04358 factor:1 | 1 (-2.06450) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90644 HOMO: -6.36746 LUMO: 2.13881 factor:1 | 1 (-2.16037) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.35926 HOMO: -6.37835 LUMO: 1.89935 factor:1 | 1 (-2.61319) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94154 HOMO: -7.03959 LUMO: 1.27349 factor:1 | 1 (-2.19547) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.12603 HOMO: -6.67495 LUMO: -0.89253 factor:1 | 1 (-3.37995) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57826 HOMO: -6.71849 LUMO: -0.97961 factor:1 | 1 (-2.83219) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94638 HOMO: -6.47903 LUMO: 0.01633 factor:1 | 1 (-2.20031) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.25145 HOMO: -6.38379 LUMO: 0.01088 factor:1 | 1 (-2.50538) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02327 HOMO: -6.49536 LUMO: -0.55239 factor:1 | 1 (-1.27719) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25859 HOMO: -6.53345 LUMO: -0.53879 factor:1 | 1 (-1.51252) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44026 HOMO: -6.16610 LUMO: 2.15514 factor:1 | 1 (-0.69419) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86315 HOMO: -6.35114 LUMO: 1.98643 factor:1 | 1 (-1.11708) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11507.26265 HOMO: -6.43277 LUMO: 2.16058 factor:1 | -1 (2.48342) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.25883 HOMO: -6.89809 LUMO: 2.20684 factor:1 | -1 (1.48724) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11507.98307 HOMO: -6.54434 LUMO: 1.93473 factor:1 | -1 (1.76300) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11507.92422 HOMO: -6.72938 LUMO: 2.03269 factor:1 | -1 (1.82186) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95915 HOMO: -6.90353 LUMO: 2.19868 factor:1 | 1 (-2.21307) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60925 HOMO: -6.41372 LUMO: 2.02453 factor:1 | 1 (-2.86318) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.32476 HOMO: -6.46543 LUMO: 1.90752 factor:1 | 1 (-2.57869) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.05647 HOMO: -6.55522 LUMO: 2.11977 factor:1 | 1 (-0.31040) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65616 HOMO: -6.28855 LUMO: 2.02181 factor:1 | 1 (-0.91008) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36559 HOMO: -6.45726 LUMO: 1.52112 factor:1 | 1 (-0.61952) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.24704 HOMO: -6.37291 LUMO: 2.11705 factor:1 | -1 (0.49903) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.78458 HOMO: -6.88448 LUMO: 2.24494 factor:1 | 1 (-0.03850) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.40397 HOMO: -6.86271 LUMO: 2.41637 factor:1 | -1 (0.34210) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34709 HOMO: -6.69400 LUMO: 2.34562 factor:1 | 1 (-0.60102) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76206 HOMO: -6.18243 LUMO: 2.53882 factor:1 | 1 (-1.01599) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48673 HOMO: -6.61237 LUMO: 2.54154 factor:1 | 1 (-1.74066) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34750 HOMO: -6.69672 LUMO: 2.16331 factor:1 | 1 (-0.60143) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39449 HOMO: -6.33481 LUMO: 2.34018 factor:1 | 1 (-0.64842) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41844 HOMO: -5.99739 LUMO: 2.37283 factor:1 | 1 (-0.67237) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30928 HOMO: -6.49808 LUMO: 2.47351 factor:1 | 1 (-1.56321) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43005 HOMO: -6.22052 LUMO: 1.86398 factor:1 | 1 (-1.68398) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11440 HOMO: -6.32665 LUMO: 2.28031 factor:1 | 1 (-1.36832) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27598 HOMO: -5.98378 LUMO: 2.16331 factor:1 | 1 (-1.52991) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.06575 HOMO: -6.08991 LUMO: 2.30208 factor:1 | 1 (-3.31968) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.63685 HOMO: -7.07224 LUMO: 1.55105 factor:1 | 1 (-2.89077) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60349 HOMO: -6.84638 LUMO: 1.76874 factor:1 | 1 (-2.85741) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46823 HOMO: -6.68856 LUMO: 1.47758 factor:1 | 1 (-0.72216) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19362 HOMO: -6.69672 LUMO: 1.71976 factor:1 | 1 (-0.44755) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55360 HOMO: -6.86543 LUMO: 2.24766 factor:1 | 1 (-0.80753) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83115 HOMO: -7.21646 LUMO: 1.71976 factor:1 | 1 (-1.08508) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63237 HOMO: -6.94162 LUMO: 2.21773 factor:1 | 1 (-0.88630) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70527 HOMO: -6.34842 LUMO: 2.04358 factor:1 | 1 (-0.95920) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73610 HOMO: -6.53345 LUMO: 1.96738 factor:1 | 1 (-0.99003) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18525 HOMO: -6.34842 LUMO: 1.88303 factor:1 | 1 (-1.43918) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72595 HOMO: -6.38651 LUMO: 2.08983 factor:1 | 1 (-0.97988) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75727 HOMO: -6.01372 LUMO: 1.43676 factor:1 | 1 (-2.01119) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.18252 HOMO: -6.30216 LUMO: 1.41771 factor:1 | 1 (-3.43644) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31758 HOMO: -6.52801 LUMO: 1.77146 factor:1 | 1 (-2.57150) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.59870 HOMO: -6.53617 LUMO: 1.72792 factor:1 | 1 (-2.85262) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21562 HOMO: -6.56611 LUMO: 2.20412 factor:1 | 1 (-1.46955) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27815 HOMO: -6.66679 LUMO: -0.72927 factor:1 | 1 (-1.53208) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56804 HOMO: -6.85455 LUMO: -0.85444 factor:1 | 1 (-1.82197) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70388 HOMO: -7.21646 LUMO: 0.27211 factor:1 | 1 (-1.95780) | 1 | 1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12454 HOMO: -6.57971 LUMO: -0.41361 factor:1 | 1 (-2.37847) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72472 HOMO: -7.03142 LUMO: -1.14288 factor:1 | 1 (-1.97865) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51372 HOMO: -6.29944 LUMO: 0.06803 factor:1 | 1 (-1.76765) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71667 HOMO: -6.47359 LUMO: 0.28028 factor:1 | 1 (-1.97059) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77533 HOMO: -6.42189 LUMO: 1.61364 factor:1 | 1 (-2.02926) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54997 HOMO: -6.41100 LUMO: 1.80956 factor:1 | 1 (-1.80390) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52684 HOMO: -6.83278 LUMO: 1.83949 factor:1 | 1 (-1.78077) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75569 HOMO: -6.78380 LUMO: -0.76192 factor:1 | 1 (-2.00962) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66012 HOMO: -6.95795 LUMO: 2.13609 factor:1 | 1 (-1.91405) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83865 HOMO: -6.57155 LUMO: 1.89119 factor:1 | 1 (-2.09258) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56436 HOMO: -6.65591 LUMO: 1.93745 factor:1 | 1 (-2.81828) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95409 HOMO: -6.44638 LUMO: 2.26943 factor:1 | 1 (-2.20801) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.36788 HOMO: -5.88038 LUMO: 1.90480 factor:1 | 1 (-3.62181) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.87427 HOMO: -6.22052 LUMO: 2.17691 factor:1 | 1 (-3.12819) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.37991 HOMO: -6.04637 LUMO: 2.23950 factor:1 | 1 (-3.63384) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79101 HOMO: -6.44366 LUMO: 2.24766 factor:1 | 1 (-2.04494) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.87247 HOMO: -6.81917 LUMO: 2.08439 factor:1 | 1 (-3.12640) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.06089 HOMO: -6.48447 LUMO: 2.28576 factor:1 | 1 (-2.31482) | -1 | -1 |
| G: -5245.38038 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72490 HOMO: -6.54434 LUMO: 1.99187 factor:1 | 1 (-2.97883) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51083 HOMO: -6.17698 LUMO: -0.65852 factor:1 | 1 (-2.76476) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.35523 HOMO: -6.08174 LUMO: -0.58504 factor:1 | 1 (-3.60915) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68577 HOMO: -6.55250 LUMO: -0.86804 factor:1 | 1 (-2.93970) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.72002 HOMO: -6.57699 LUMO: -0.89525 factor:1 | 1 (-3.97395) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.61433 HOMO: -6.63141 LUMO: -1.04220 factor:1 | 1 (-3.86826) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.02360 HOMO: -6.69128 LUMO: -0.76736 factor:1 | 1 (-3.27753) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.82217 HOMO: -6.25318 LUMO: -1.03131 factor:1 | 1 (-1.07610) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64455 HOMO: -6.69944 LUMO: 0.01905 factor:1 | 1 (-2.89848) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.66468 HOMO: -6.28583 LUMO: 0.38368 factor:1 | 1 (-2.91861) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71956 HOMO: -6.90081 LUMO: -0.83811 factor:1 | 1 (-0.97349) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.58531 HOMO: -6.78380 LUMO: -0.10068 factor:1 | 1 (-2.83924) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.58542 HOMO: -6.30488 LUMO: -0.98505 factor:1 | -1 (0.16066) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.32560 HOMO: -6.29671 LUMO: -1.79051 factor:1 | -1 (0.42047) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.63527 HOMO: -6.76747 LUMO: -0.22041 factor:1 | 1 (-2.88920) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.10198 HOMO: -6.22597 LUMO: -0.94968 factor:1 | 1 (-2.35591) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88962 HOMO: -6.73482 LUMO: 0.05987 factor:1 | 1 (-2.14355) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59191 HOMO: -6.28855 LUMO: 0.34831 factor:1 | 1 (-0.84584) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35623 HOMO: -6.69400 LUMO: 0.25307 factor:1 | 1 (-0.61016) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.22428 HOMO: -6.70216 LUMO: 0.61226 factor:1 | 1 (-0.47821) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.66912 HOMO: -6.70216 LUMO: 0.17415 factor:1 | 1 (-2.92305) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80418 HOMO: -6.70761 LUMO: 0.24762 factor:1 | 1 (-2.05811) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.11787 HOMO: -6.68856 LUMO: -0.84900 factor:1 | 1 (-2.37180) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.11240 HOMO: -6.71033 LUMO: -0.38640 factor:1 | 1 (-2.36633) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65615 HOMO: -6.24501 LUMO: -0.09252 factor:1 | 1 (-1.91008) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62076 HOMO: -6.81645 LUMO: -0.07347 factor:1 | 1 (-2.87469) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21868 HOMO: -6.49536 LUMO: 0.09796 factor:1 | 1 (-0.47261) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55345 HOMO: -6.71033 LUMO: -0.26395 factor:1 | 1 (-1.80738) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50725 HOMO: -6.70489 LUMO: -0.09252 factor:1 | 1 (-1.76118) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71365 HOMO: -6.23685 LUMO: 0.39729 factor:1 | 1 (-1.96757) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79455 HOMO: -6.69400 LUMO: -0.05442 factor:1 | 1 (-2.04847) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99844 HOMO: -6.36202 LUMO: 0.09796 factor:1 | 1 (-2.25237) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.01414 HOMO: -6.54978 LUMO: 0.15510 factor:1 | 1 (-2.26807) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80663 HOMO: -6.77836 LUMO: 0.25851 factor:1 | 1 (-2.06055) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23377 HOMO: -5.70623 LUMO: 0.73471 factor:1 | 1 (-1.48770) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28267 HOMO: -5.58378 LUMO: 0.89253 factor:1 | 1 (-1.53660) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35486 HOMO: -5.68718 LUMO: 0.87893 factor:1 | 1 (-1.60879) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62310 HOMO: -5.10486 LUMO: 1.11567 factor:1 | 1 (-2.87703) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78282 HOMO: -4.59328 LUMO: 1.27621 factor:1 | 1 (-2.03675) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87999 HOMO: -4.45450 LUMO: 1.82044 factor:1 | 1 (-2.13392) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86683 HOMO: -4.64226 LUMO: 1.70615 factor:1 | 1 (-1.12076) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08460 HOMO: -5.04227 LUMO: 1.04492 factor:1 | 1 (-1.33853) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36660 HOMO: -4.85723 LUMO: 0.93607 factor:1 | 1 (-0.62053) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41340 HOMO: -4.72934 LUMO: 1.00410 factor:1 | 1 (-0.66733) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17468 HOMO: -4.56335 LUMO: 1.56738 factor:1 | 1 (-0.42861) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.24635 HOMO: -5.48854 LUMO: 0.33198 factor:1 | 1 (-0.50028) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60270 HOMO: -4.97424 LUMO: 1.33608 factor:1 | 1 (-2.85662) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94111 HOMO: -4.60145 LUMO: 1.74697 factor:1 | 1 (-2.19503) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89147 HOMO: -5.60010 LUMO: 0.74831 factor:1 | 1 (-2.14540) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52232 HOMO: -5.66541 LUMO: 0.66668 factor:1 | 1 (-1.77625) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49865 HOMO: -6.50080 LUMO: 0.07075 factor:1 | 1 (-1.75258) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66622 HOMO: -5.79603 LUMO: 0.22313 factor:1 | 1 (-1.92014) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92445 HOMO: -4.68036 LUMO: 1.29798 factor:1 | 1 (-2.17838) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92530 HOMO: -4.84363 LUMO: 1.34424 factor:1 | 1 (-2.17922) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.24215 HOMO: -4.62321 LUMO: 1.82861 factor:1 | 1 (-2.49607) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93800 HOMO: -5.83684 LUMO: 0.82178 factor:1 | 1 (-2.19193) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86777 HOMO: -5.27629 LUMO: 0.57960 factor:1 | 1 (-2.12170) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.47788 HOMO: -5.15928 LUMO: -2.96876 factor:1 | 1 (-2.73181) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48114 HOMO: -5.08853 LUMO: 0.89253 factor:1 | 1 (-2.73507) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65540 HOMO: -6.42461 LUMO: 0.04354 factor:1 | 1 (-2.90933) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74551 HOMO: -6.42733 LUMO: -0.00544 factor:1 | 1 (-1.99944) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.05529 HOMO: -5.87494 LUMO: 0.69933 factor:1 | 1 (-1.30922) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04297 HOMO: -5.07492 LUMO: 1.02587 factor:1 | 1 (-1.29689) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12708 HOMO: -4.44362 LUMO: 1.99187 factor:1 | 1 (-1.38101) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.93691 HOMO: -5.82052 LUMO: 0.43810 factor:1 | 1 (-3.19083) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04411 HOMO: -5.75793 LUMO: 0.76464 factor:1 | 1 (-1.29804) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.65752 HOMO: -5.09669 LUMO: 0.72382 factor:1 | 1 (-3.91145) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.17819 HOMO: -6.75387 LUMO: -2.02453 factor:1 | 1 (-3.43212) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65887 HOMO: -5.02322 LUMO: 1.14832 factor:1 | 1 (-1.91280) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56180 HOMO: -5.75521 LUMO: 0.73471 factor:1 | 1 (-2.81573) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85871 HOMO: -5.89943 LUMO: 0.54967 factor:1 | 1 (-2.11264) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.99242 HOMO: -5.80147 LUMO: 0.72382 factor:1 | 1 (-3.24635) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.37841 HOMO: -6.16066 LUMO: 0.39457 factor:1 | 1 (-3.63234) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.48971 HOMO: -5.98650 LUMO: 0.76736 factor:1 | 1 (-3.74363) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.90556 HOMO: -4.74839 LUMO: 1.88847 factor:1 | 1 (-3.15949) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.14026 HOMO: -5.62459 LUMO: 0.26939 factor:1 | 1 (-3.39419) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27081 HOMO: -4.88172 LUMO: 1.30070 factor:1 | 1 (-1.52474) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43021 HOMO: -5.09397 LUMO: 0.98505 factor:1 | 1 (-1.68414) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17140 HOMO: -6.50080 LUMO: -0.28300 factor:1 | 1 (-1.42533) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.81957 HOMO: -5.04227 LUMO: 1.49935 factor:1 | 1 (-3.07350) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.90477 HOMO: -5.22731 LUMO: 0.88437 factor:1 | 1 (-3.15870) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.74628 HOMO: -4.95519 LUMO: 1.25717 factor:1 | 1 (-1.00021) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.82911 HOMO: -4.61233 LUMO: 1.27621 factor:1 | 1 (-1.08304) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76410 HOMO: -4.70757 LUMO: 1.63813 factor:1 | 1 (-1.01803) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59256 HOMO: -4.85179 LUMO: 1.11839 factor:1 | 1 (-0.84649) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.82670 HOMO: -4.97696 LUMO: 1.00138 factor:1 | 1 (-3.08063) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01362 HOMO: -5.64636 LUMO: 0.81090 factor:1 | 1 (-3.26754) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.92937 HOMO: -4.37831 LUMO: 1.90208 factor:1 | 1 (-3.18330) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.27710 HOMO: -4.67764 LUMO: 1.54561 factor:1 | 1 (-3.53103) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24264 HOMO: -5.87766 LUMO: 0.42994 factor:1 | 1 (-1.49657) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19336 HOMO: -6.03821 LUMO: 0.32382 factor:1 | 1 (-1.44729) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.16683 HOMO: -5.99739 LUMO: 0.69389 factor:1 | 1 (-1.42076) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.23779 HOMO: -6.43821 LUMO: 0.15238 factor:1 | -1 (0.50828) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.51676 HOMO: -6.63414 LUMO: -0.07347 factor:1 | -1 (0.22931) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.66343 HOMO: -6.50080 LUMO: 0.10068 factor:1 | -1 (0.08264) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.96169 HOMO: -6.49264 LUMO: 0.19592 factor:1 | 1 (-0.21562) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.15993 HOMO: -5.83956 LUMO: 0.12517 factor:1 | 1 (-0.41386) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33351 HOMO: -6.50896 LUMO: 0.19048 factor:1 | 1 (-0.58744) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51155 HOMO: -6.56611 LUMO: 0.04898 factor:1 | 1 (-1.76547) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77697 HOMO: -6.68040 LUMO: -0.08436 factor:1 | 1 (-2.03089) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89188 HOMO: -6.73754 LUMO: -0.08708 factor:1 | 1 (-2.14581) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.06677 HOMO: -6.80285 LUMO: -0.10612 factor:1 | 1 (-2.32070) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.18851 HOMO: -6.35658 LUMO: 0.02177 factor:1 | 1 (-2.44244) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.40740 HOMO: -5.74160 LUMO: 0.14694 factor:1 | 1 (-2.66133) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22338 HOMO: -4.78376 LUMO: 0.92791 factor:1 | 1 (-1.47731) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36741 HOMO: -5.90215 LUMO: 0.36463 factor:1 | 1 (-1.62134) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22022 HOMO: -4.99329 LUMO: 0.85988 factor:1 | 1 (-1.47415) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72807 HOMO: -4.93887 LUMO: 1.33608 factor:1 | 1 (-1.98200) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.73932 HOMO: -5.19193 LUMO: 0.50341 factor:1 | 1 (-2.99325) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79947 HOMO: -6.64502 LUMO: -1.98643 factor:1 | 1 (-2.05340) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.35202 HOMO: -5.15384 LUMO: 0.94968 factor:1 | 1 (-2.60595) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.40683 HOMO: -6.31032 LUMO: 0.08436 factor:1 | 1 (-2.66076) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54348 HOMO: -4.88716 LUMO: 0.82995 factor:1 | 1 (-2.79741) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53068 HOMO: -5.57017 LUMO: 0.19320 factor:1 | 1 (-1.78460) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82287 HOMO: -4.92254 LUMO: 0.93879 factor:1 | 1 (-2.07680) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86630 HOMO: -4.77288 LUMO: 1.60003 factor:1 | 1 (-2.12023) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.63633 HOMO: -4.97696 LUMO: 0.89798 factor:1 | 1 (-2.89026) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.07240 HOMO: -5.00690 LUMO: 1.14288 factor:1 | 1 (-2.32633) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42621 HOMO: -4.88444 LUMO: 1.48574 factor:1 | 1 (-1.68014) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57666 HOMO: -5.03955 LUMO: 1.51023 factor:1 | 1 (-1.83059) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39364 HOMO: -5.22459 LUMO: 0.99049 factor:1 | 1 (-1.64757) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.62302 HOMO: -5.29534 LUMO: 0.96056 factor:1 | -1 (0.12305) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.56920 HOMO: -5.35520 LUMO: 0.68301 factor:1 | -1 (0.17687) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27879 HOMO: -5.27357 LUMO: 1.18642 factor:1 | 1 (-0.53272) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.18559 HOMO: -5.79875 LUMO: 0.61770 factor:1 | 1 (-0.43952) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49248 HOMO: -7.64640 LUMO: -2.45175 factor:1 | 1 (-0.74641) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.26244 HOMO: -7.46953 LUMO: -1.29798 factor:1 | 1 (-0.51636) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.11315 HOMO: -7.95389 LUMO: -0.37280 factor:1 | 1 (-0.36708) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52266 HOMO: -7.23279 LUMO: -1.19186 factor:1 | 1 (-0.77659) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56953 HOMO: -7.14299 LUMO: -1.12927 factor:1 | 1 (-1.82346) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56265 HOMO: -6.93074 LUMO: 0.31565 factor:1 | 1 (-1.81658) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.39355 HOMO: -6.63141 LUMO: 0.28028 factor:1 | -1 (0.35252) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.29183 HOMO: -7.10489 LUMO: -1.07213 factor:1 | -1 (0.45424) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.07402 HOMO: -7.00693 LUMO: -0.69389 factor:1 | 1 (-0.32795) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.96531 HOMO: -8.50356 LUMO: -1.79595 factor:1 | 1 (-0.21924) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65293 HOMO: -7.79334 LUMO: -2.33746 factor:1 | 1 (-2.90686) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85368 HOMO: -7.24367 LUMO: -0.85172 factor:1 | 1 (-2.10760) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78641 HOMO: -7.94028 LUMO: -0.20136 factor:1 | 1 (-2.04034) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23230 HOMO: -7.22462 LUMO: 0.84627 factor:1 | 1 (-1.48623) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55168 HOMO: -6.54978 LUMO: 0.34831 factor:1 | 1 (-1.80561) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43908 HOMO: -6.86815 LUMO: 0.32109 factor:1 | 1 (-1.69301) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.30508 HOMO: -7.17564 LUMO: -1.28438 factor:1 | 1 (-0.55900) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21803 HOMO: -7.03142 LUMO: -1.12655 factor:1 | 1 (-0.47195) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29305 HOMO: -7.39878 LUMO: 0.15783 factor:1 | 1 (-0.54698) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.15185 HOMO: -7.25728 LUMO: 0.42178 factor:1 | 1 (-0.40578) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50131 HOMO: -6.86543 LUMO: 0.93879 factor:1 | 1 (-2.75523) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63351 HOMO: -7.09673 LUMO: -0.69661 factor:1 | 1 (-1.88744) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80323 HOMO: -7.74708 LUMO: 0.01088 factor:1 | 1 (-2.05715) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73705 HOMO: -6.80557 LUMO: 0.46531 factor:1 | 1 (-1.99098) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53381 HOMO: -7.29265 LUMO: 1.31975 factor:1 | 1 (-1.78773) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57318 HOMO: -6.93618 LUMO: 0.29388 factor:1 | 1 (-1.82711) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54181 HOMO: -6.53073 LUMO: 0.71022 factor:1 | 1 (-1.79573) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38588 HOMO: -6.41917 LUMO: -1.24084 factor:1 | 1 (-1.63981) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75773 HOMO: -6.67495 LUMO: -1.09118 factor:1 | 1 (-2.01166) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67310 HOMO: -6.97156 LUMO: -0.53606 factor:1 | 1 (-1.92703) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50036 HOMO: -6.85183 LUMO: -0.45715 factor:1 | 1 (-1.75429) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57419 HOMO: -7.12666 LUMO: -0.67484 factor:1 | 1 (-1.82812) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60597 HOMO: -7.49946 LUMO: -0.14694 factor:1 | 1 (-1.85990) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43209 HOMO: -7.44231 LUMO: 0.58232 factor:1 | 1 (-1.68602) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36553 HOMO: -7.36340 LUMO: -0.68301 factor:1 | 1 (-1.61946) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48602 HOMO: -6.13073 LUMO: -0.54967 factor:1 | 1 (-1.73995) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45472 HOMO: -7.81511 LUMO: -0.06531 factor:1 | 1 (-2.70865) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54134 HOMO: -7.26816 LUMO: -1.02587 factor:1 | 1 (-1.79527) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52893 HOMO: -7.98110 LUMO: -0.17960 factor:1 | 1 (-1.78286) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66056 HOMO: -7.44776 LUMO: -1.00954 factor:1 | 1 (-1.91448) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.25139 HOMO: -7.47769 LUMO: -1.02859 factor:1 | 1 (-0.50532) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.20377 HOMO: -6.75659 LUMO: 0.39457 factor:1 | 1 (-0.45770) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38761 HOMO: -6.71849 LUMO: 0.36735 factor:1 | 1 (-0.64154) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48755 HOMO: -7.64096 LUMO: -1.43948 factor:1 | 1 (-0.74148) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73294 HOMO: -7.83144 LUMO: -1.36601 factor:1 | 1 (-1.98687) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71449 HOMO: -7.19469 LUMO: 0.35103 factor:1 | 1 (-1.96842) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03101 HOMO: -7.03414 LUMO: 0.20409 factor:1 | 1 (-2.28494) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08435 HOMO: -7.22734 LUMO: 0.31293 factor:1 | 1 (-2.33827) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.25923 HOMO: -6.93618 LUMO: 0.56055 factor:1 | 1 (-2.51316) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.37594 HOMO: -6.94707 LUMO: -0.88709 factor:1 | 1 (-2.62987) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39761 HOMO: -6.86543 LUMO: -0.83267 factor:1 | 1 (-1.65154) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31405 HOMO: -6.82189 LUMO: -1.15376 factor:1 | 1 (-1.56797) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48254 HOMO: -6.65046 LUMO: -0.46531 factor:1 | 1 (-1.73647) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61862 HOMO: -6.52529 LUMO: 0.20953 factor:1 | 1 (-1.87255) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27114 HOMO: -6.80557 LUMO: 0.44355 factor:1 | 1 (-0.52507) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25184 HOMO: -6.93074 LUMO: -0.81634 factor:1 | 1 (-1.50577) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70244 HOMO: -7.43143 LUMO: -0.45987 factor:1 | 1 (-0.95637) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99159 HOMO: -7.07224 LUMO: -0.68028 factor:1 | 1 (-1.24552) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78959 HOMO: -6.68040 LUMO: -0.71566 factor:1 | 1 (-2.04352) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33900 HOMO: -6.26406 LUMO: -1.09934 factor:1 | 1 (-1.59293) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65870 HOMO: -5.94569 LUMO: -0.72110 factor:1 | 1 (-2.91263) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.36593 HOMO: -6.12256 LUMO: -0.42178 factor:1 | 1 (-2.61986) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86968 HOMO: -6.09807 LUMO: 0.11429 factor:1 | 1 (-2.12360) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21165 HOMO: -7.35252 LUMO: -0.55783 factor:1 | 1 (-1.46558) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20479 HOMO: -7.57837 LUMO: -0.76736 factor:1 | 1 (-1.45872) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44014 HOMO: -6.16066 LUMO: 0.01905 factor:1 | 1 (-1.69407) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.09642 HOMO: -6.13345 LUMO: -0.41906 factor:1 | 1 (-3.35035) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.61483 HOMO: -6.10351 LUMO: -0.33742 factor:1 | 1 (-2.86876) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68425 HOMO: -7.24639 LUMO: -0.51702 factor:1 | 1 (-2.93818) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49831 HOMO: -6.98244 LUMO: -1.82044 factor:1 | 1 (-2.75224) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.13558 HOMO: -6.37563 LUMO: -1.67622 factor:1 | 1 (-3.38950) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.70019 HOMO: -5.79058 LUMO: -2.55243 factor:1 | 1 (-2.95412) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55884 HOMO: -6.34025 LUMO: -0.27483 factor:1 | 1 (-1.81277) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.11054 HOMO: -6.05453 LUMO: -0.51157 factor:1 | 1 (-0.36447) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47313 HOMO: -7.53755 LUMO: -0.38912 factor:1 | 1 (-0.72706) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.40677 HOMO: -7.00421 LUMO: -0.50885 factor:1 | 1 (-3.66069) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.38283 HOMO: -7.52123 LUMO: -0.37552 factor:1 | 1 (-2.63676) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50847 HOMO: -6.70489 LUMO: -1.04764 factor:1 | 1 (-1.76240) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38169 HOMO: -7.06408 LUMO: -1.16737 factor:1 | 1 (-1.63562) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44735 HOMO: -6.71849 LUMO: -1.02315 factor:1 | 1 (-1.70128) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69147 HOMO: -6.16610 LUMO: -0.50885 factor:1 | 1 (-1.94540) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66847 HOMO: -6.48447 LUMO: 0.07619 factor:1 | 1 (-1.92240) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49556 HOMO: -7.06135 LUMO: 0.09796 factor:1 | 1 (-2.74949) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69242 HOMO: -6.47359 LUMO: 0.22585 factor:1 | 1 (-1.94635) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80216 HOMO: -6.10896 LUMO: -0.62314 factor:1 | 1 (-2.05609) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.36680 HOMO: -6.88176 LUMO: -0.96600 factor:1 | 1 (-2.62073) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26065 HOMO: -6.67495 LUMO: 0.21769 factor:1 | 1 (-2.51458) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89855 HOMO: -6.84911 LUMO: 0.38368 factor:1 | 1 (-2.15248) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.19134 HOMO: -6.83550 LUMO: 1.29798 factor:1 | 1 (-2.44527) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.33668 HOMO: -6.67495 LUMO: 1.46941 factor:1 | 1 (-2.59061) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49367 HOMO: -6.81917 LUMO: 1.30887 factor:1 | 1 (-1.74760) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57947 HOMO: -6.56611 LUMO: 0.66396 factor:1 | 1 (-1.83339) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51614 HOMO: -6.76203 LUMO: 0.60137 factor:1 | 1 (-2.77006) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.82129 HOMO: -6.55794 LUMO: 0.34286 factor:1 | 1 (-3.07521) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19773 HOMO: -6.83550 LUMO: 0.35919 factor:1 | 1 (-0.45165) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.22110 HOMO: -7.17836 LUMO: 0.63130 factor:1 | 1 (-0.47503) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.44252 HOMO: -6.29944 LUMO: -0.69389 factor:1 | 1 (-3.69645) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.44307 HOMO: -7.06680 LUMO: -0.95784 factor:1 | 1 (-2.69700) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.53916 HOMO: -6.84638 LUMO: -0.87076 factor:1 | 1 (-2.79309) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.78934 HOMO: -6.96339 LUMO: -1.05308 factor:1 | 1 (-3.04327) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22077 HOMO: -6.75387 LUMO: -1.04220 factor:1 | 1 (-1.47469) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99897 HOMO: -6.71849 LUMO: -0.84355 factor:1 | 1 (-1.25289) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10112 HOMO: -7.16748 LUMO: 0.51702 factor:1 | 1 (-1.35505) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27775 HOMO: -6.92530 LUMO: 0.71566 factor:1 | 1 (-1.53167) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20120 HOMO: -7.11034 LUMO: 0.01905 factor:1 | 1 (-1.45513) | 1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22468 HOMO: -6.79468 LUMO: 0.77008 factor:1 | 1 (-1.47861) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.09601 HOMO: -6.52801 LUMO: 0.98233 factor:1 | 1 (-0.34994) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46614 HOMO: -6.76475 LUMO: 0.53334 factor:1 | 1 (-0.72007) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.23841 HOMO: -5.29261 LUMO: 0.57416 factor:1 | 1 (-0.49234) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21524 HOMO: -6.57971 LUMO: 0.12789 factor:1 | 1 (-1.46917) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99143 HOMO: -6.99333 LUMO: 0.51430 factor:1 | 1 (-1.24536) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25873 HOMO: -6.41917 LUMO: 0.19048 factor:1 | 1 (-1.51265) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09736 HOMO: -6.16066 LUMO: 1.77146 factor:1 | 1 (-1.35129) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21347 HOMO: -6.90353 LUMO: 1.65717 factor:1 | 1 (-1.46740) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36273 HOMO: -5.94569 LUMO: 1.29526 factor:1 | 1 (-1.61666) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.08790 HOMO: -6.60420 LUMO: 1.33880 factor:1 | 1 (-0.34183) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34162 HOMO: -6.23957 LUMO: 0.09524 factor:1 | 1 (-0.59555) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.26320 HOMO: -6.80013 LUMO: 1.34696 factor:1 | 1 (-0.51713) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38510 HOMO: -7.53483 LUMO: -1.52384 factor:1 | 1 (-1.63902) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34825 HOMO: -7.62463 LUMO: -1.65717 factor:1 | 1 (-1.60218) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46986 HOMO: -7.62463 LUMO: -1.61364 factor:1 | 1 (-1.72379) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03472 HOMO: -8.04096 LUMO: -1.66806 factor:1 | 1 (-1.28865) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86977 HOMO: -7.18381 LUMO: -1.17553 factor:1 | 1 (-1.12369) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89050 HOMO: -7.69538 LUMO: -1.36601 factor:1 | 1 (-1.14443) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99771 HOMO: -7.95117 LUMO: -1.48302 factor:1 | 1 (-1.25164) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06974 HOMO: -6.98516 LUMO: 0.35919 factor:1 | 1 (-1.32367) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.05908 HOMO: -7.91579 LUMO: -0.32109 factor:1 | 1 (-1.31300) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11407 HOMO: -6.75659 LUMO: -0.03537 factor:1 | 1 (-1.36800) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81656 HOMO: -7.78518 LUMO: -2.36467 factor:1 | 1 (-2.07049) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.11523 HOMO: -7.96477 LUMO: -2.75651 factor:1 | 1 (-2.36916) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61011 HOMO: -7.60286 LUMO: -2.35106 factor:1 | 1 (-1.86403) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79689 HOMO: -7.38245 LUMO: -1.21635 factor:1 | 1 (-2.05081) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90998 HOMO: -7.91579 LUMO: -1.50479 factor:1 | 1 (-2.16390) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65532 HOMO: -8.07362 LUMO: -0.28028 factor:1 | 1 (-2.90925) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51548 HOMO: -7.38245 LUMO: -1.15921 factor:1 | 1 (-2.76941) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.41363 HOMO: -7.18653 LUMO: -0.94968 factor:1 | 1 (-2.66756) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.65945 HOMO: -6.88448 LUMO: 0.38096 factor:1 | 1 (-3.91338) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.69883 HOMO: -6.97972 LUMO: 0.43266 factor:1 | 1 (-2.95276) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.06692 HOMO: -6.88992 LUMO: -0.43538 factor:1 | 1 (-3.32085) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45690 HOMO: -7.97021 LUMO: -0.17143 factor:1 | 1 (-2.71083) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.59804 HOMO: -6.92530 LUMO: 0.77280 factor:1 | 1 (-2.85197) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51059 HOMO: -7.89674 LUMO: -0.09796 factor:1 | 1 (-2.76451) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72647 HOMO: -7.02870 LUMO: 0.88709 factor:1 | 1 (-0.98040) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79771 HOMO: -6.78380 LUMO: 0.22041 factor:1 | 1 (-1.05164) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79142 HOMO: -7.24911 LUMO: -0.82178 factor:1 | 1 (-1.04535) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.88692 HOMO: -6.77019 LUMO: 0.52790 factor:1 | 1 (-0.14085) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.11843 HOMO: -8.56070 LUMO: -1.83405 factor:1 | 1 (-0.37236) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.06428 HOMO: -7.74164 LUMO: -2.36195 factor:1 | 1 (-0.31821) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.93690 HOMO: -7.39878 LUMO: -2.41637 factor:1 | 1 (-1.19082) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08131 HOMO: -7.61647 LUMO: -2.34018 factor:1 | 1 (-1.33524) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89558 HOMO: -6.93346 LUMO: -0.57688 factor:1 | 1 (-2.14951) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12350 HOMO: -6.85183 LUMO: -1.00410 factor:1 | 1 (-2.37743) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.41061 HOMO: -7.18925 LUMO: -1.12655 factor:1 | 1 (-2.66454) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.40419 HOMO: -6.85183 LUMO: -1.60275 factor:1 | 1 (-2.65812) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.74624 HOMO: -7.51578 LUMO: 0.12517 factor:1 | 1 (-0.00016) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.02080 HOMO: -7.36068 LUMO: 0.05714 factor:1 | 1 (-0.27473) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88320 HOMO: -7.49674 LUMO: 0.18776 factor:1 | 1 (-2.13713) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85539 HOMO: -7.09401 LUMO: -1.24900 factor:1 | 1 (-2.10932) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03289 HOMO: -7.22462 LUMO: -1.61364 factor:1 | 1 (-2.28682) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08364 HOMO: -7.74436 LUMO: -0.18776 factor:1 | 1 (-2.33757) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.39015 HOMO: -7.35252 LUMO: 0.75376 factor:1 | 1 (-2.64408) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.06602 HOMO: -7.75252 LUMO: 0.00816 factor:1 | 1 (-3.31995) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55001 HOMO: -7.06680 LUMO: 0.24490 factor:1 | 1 (-2.80394) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64447 HOMO: -7.49129 LUMO: 0.14150 factor:1 | 1 (-2.89839) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81199 HOMO: -6.90625 LUMO: -1.11295 factor:1 | 1 (-2.06592) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94636 HOMO: -6.78380 LUMO: -0.93063 factor:1 | 1 (-2.20029) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97950 HOMO: -7.79878 LUMO: 0.30477 factor:1 | 1 (-2.23343) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99219 HOMO: -7.87498 LUMO: 0.61770 factor:1 | 1 (-1.24612) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13853 HOMO: -7.23823 LUMO: 0.30205 factor:1 | 1 (-1.39246) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33024 HOMO: -7.67633 LUMO: 0.13061 factor:1 | 1 (-1.58417) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44700 HOMO: -7.79606 LUMO: 0.34558 factor:1 | 1 (-1.70093) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10774 HOMO: -6.66135 LUMO: -2.60141 factor:1 | 1 (-0.36167) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33732 HOMO: -7.03142 LUMO: 0.50885 factor:1 | 1 (-0.59125) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96726 HOMO: -7.05591 LUMO: -0.06531 factor:1 | 1 (-1.22119) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.94882 HOMO: -7.45592 LUMO: -1.39594 factor:1 | 1 (-1.20274) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.98155 HOMO: -7.22462 LUMO: -1.10478 factor:1 | 1 (-1.23548) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01524 HOMO: -8.14709 LUMO: -0.55783 factor:1 | 1 (-1.26917) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.82245 HOMO: -7.22190 LUMO: -1.14560 factor:1 | 1 (-1.07637) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89230 HOMO: -7.28721 LUMO: -1.14016 factor:1 | 1 (-1.14623) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60171 HOMO: -6.97156 LUMO: 0.51702 factor:1 | 1 (-0.85563) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.89897 HOMO: -7.37156 LUMO: 0.29388 factor:1 | 1 (-0.15290) | 1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.59143 HOMO: -7.66273 LUMO: -1.59731 factor:1 | -1 (0.15464) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.20867 HOMO: -7.50490 LUMO: -1.49935 factor:1 | 1 (-0.46259) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.92656 HOMO: -7.61102 LUMO: -1.45581 factor:1 | 1 (-0.18049) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.62561 HOMO: -7.58653 LUMO: -1.61091 factor:1 | -1 (0.12046) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.85222 HOMO: -7.36068 LUMO: -1.14560 factor:1 | 1 (-0.10615) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51533 HOMO: -6.96339 LUMO: 0.26939 factor:1 | 1 (-1.76926) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63458 HOMO: -6.53617 LUMO: 0.22313 factor:1 | 1 (-0.88851) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88223 HOMO: -7.33619 LUMO: -1.02587 factor:1 | 1 (-1.13616) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.18910 HOMO: -6.87904 LUMO: 0.33742 factor:1 | 1 (-3.44303) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.10020 HOMO: -6.88448 LUMO: 0.58777 factor:1 | 1 (-3.35413) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68923 HOMO: -6.55522 LUMO: -1.51295 factor:1 | 1 (-2.94316) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.66180 HOMO: -7.43415 LUMO: 0.10612 factor:1 | 1 (-2.91573) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39103 HOMO: -7.54300 LUMO: -0.02449 factor:1 | 1 (-1.64496) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43228 HOMO: -7.42054 LUMO: 0.28028 factor:1 | 1 (-1.68621) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02626 HOMO: -6.98244 LUMO: -0.95784 factor:1 | 1 (-1.28019) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00141 HOMO: -6.96884 LUMO: -1.12383 factor:1 | 1 (-1.25534) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11532 HOMO: -6.80829 LUMO: -0.98233 factor:1 | 1 (-1.36925) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90971 HOMO: -7.60830 LUMO: 0.58504 factor:1 | 1 (-1.16364) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68744 HOMO: -7.52123 LUMO: 0.08163 factor:1 | 1 (-1.94137) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95555 HOMO: -7.59742 LUMO: 0.00272 factor:1 | 1 (-2.20948) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.05675 HOMO: -6.99333 LUMO: -1.33880 factor:1 | 1 (-2.31068) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.07699 HOMO: -6.63958 LUMO: -1.39322 factor:1 | 1 (-3.33092) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.32430 HOMO: -7.86137 LUMO: 0.01633 factor:1 | 1 (-2.57822) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57891 HOMO: -7.29537 LUMO: 0.14694 factor:1 | 1 (-2.83284) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.79187 HOMO: -6.95523 LUMO: 0.48708 factor:1 | 1 (-3.04580) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40950 HOMO: -7.10217 LUMO: -1.10478 factor:1 | 1 (-1.66343) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96724 HOMO: -6.88176 LUMO: -0.96328 factor:1 | 1 (-1.22117) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.87616 HOMO: -7.89130 LUMO: -0.13334 factor:1 | 1 (-1.13009) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.78612 HOMO: -7.75252 LUMO: 0.25579 factor:1 | 1 (-1.04005) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.68726 HOMO: -6.87632 LUMO: -0.93063 factor:1 | 1 (-0.94119) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00065 HOMO: -6.78108 LUMO: -0.86804 factor:1 | 1 (-1.25458) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.94873 HOMO: -5.98106 LUMO: 0.10340 factor:1 | 1 (-1.20266) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73624 HOMO: -6.40284 LUMO: -0.87349 factor:1 | 1 (-0.99017) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81536 HOMO: -6.77019 LUMO: -1.20819 factor:1 | 1 (-2.06929) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72366 HOMO: -6.90081 LUMO: -1.00682 factor:1 | 1 (-1.97759) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97316 HOMO: -6.59060 LUMO: -0.26667 factor:1 | 1 (-2.22709) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00541 HOMO: -6.50896 LUMO: -0.48708 factor:1 | 1 (-2.25933) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63696 HOMO: -6.20420 LUMO: -0.73471 factor:1 | 1 (-1.89089) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81553 HOMO: -6.17154 LUMO: -0.68573 factor:1 | 1 (-1.06946) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02846 HOMO: -6.21236 LUMO: 0.09796 factor:1 | 1 (-1.28239) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.19115 HOMO: -6.38379 LUMO: 0.58232 factor:1 | 1 (-2.44508) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.27866 HOMO: -7.42871 LUMO: 0.40273 factor:1 | 1 (-2.53259) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08772 HOMO: -6.54978 LUMO: 0.26395 factor:1 | 1 (-2.34165) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51769 HOMO: -7.14027 LUMO: 0.14150 factor:1 | 1 (-2.77162) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52664 HOMO: -7.25456 LUMO: -0.15783 factor:1 | 1 (-2.78057) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08685 HOMO: -6.90897 LUMO: 0.63403 factor:1 | 1 (-2.34078) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26756 HOMO: -6.49264 LUMO: 0.71022 factor:1 | 1 (-2.52149) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03384 HOMO: -6.56067 LUMO: -1.03947 factor:1 | 1 (-2.28777) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.33774 HOMO: -6.79196 LUMO: -1.12655 factor:1 | 1 (-2.59167) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.02764 HOMO: -6.95251 LUMO: -1.09118 factor:1 | 1 (-2.28157) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.09022 HOMO: -7.47225 LUMO: -0.22041 factor:1 | 1 (-2.34415) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57652 HOMO: -7.13483 LUMO: -0.98505 factor:1 | 1 (-2.83045) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.34761 HOMO: -6.99061 LUMO: -1.05852 factor:1 | 1 (-3.60154) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.81682 HOMO: -6.52257 LUMO: -1.11022 factor:1 | 1 (-3.07075) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.77650 HOMO: -6.75114 LUMO: -1.09934 factor:1 | 1 (-3.03042) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.93647 HOMO: -6.82189 LUMO: -0.89253 factor:1 | 1 (-3.19040) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71724 HOMO: -6.83278 LUMO: -0.97961 factor:1 | 1 (-1.97117) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39519 HOMO: -6.65318 LUMO: -0.84355 factor:1 | 1 (-1.64912) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55508 HOMO: -6.75931 LUMO: -0.88437 factor:1 | 1 (-1.80901) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52825 HOMO: -6.19059 LUMO: -0.45715 factor:1 | 1 (-1.78218) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43509 HOMO: -7.09673 LUMO: -2.01908 factor:1 | 1 (-0.68902) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.68171 HOMO: -7.88042 LUMO: 0.38640 factor:1 | 1 (-0.93564) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63352 HOMO: -7.83144 LUMO: 0.14422 factor:1 | 1 (-0.88744) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77284 HOMO: -7.46408 LUMO: 0.44627 factor:1 | 1 (-1.02677) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53158 HOMO: -7.12394 LUMO: -2.04902 factor:1 | 1 (-0.78551) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20319 HOMO: -6.78380 LUMO: -1.11295 factor:1 | 1 (-1.45712) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49995 HOMO: -7.12938 LUMO: -0.23674 factor:1 | 1 (-1.75388) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46999 HOMO: -6.14705 LUMO: -0.20409 factor:1 | 1 (-1.72392) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68594 HOMO: -6.50080 LUMO: -0.28300 factor:1 | 1 (-1.93987) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40262 HOMO: -6.50352 LUMO: -0.62042 factor:1 | 1 (-1.65655) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59893 HOMO: -6.46543 LUMO: -0.53879 factor:1 | 1 (-0.85286) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66040 HOMO: -7.32803 LUMO: -0.52790 factor:1 | 1 (-0.91433) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56843 HOMO: -5.94025 LUMO: -0.17687 factor:1 | 1 (-0.82236) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64595 HOMO: -5.62187 LUMO: 0.05714 factor:1 | 1 (-0.89988) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67365 HOMO: -7.03414 LUMO: -1.04492 factor:1 | 1 (-0.92758) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76038 HOMO: -6.75387 LUMO: -2.02181 factor:1 | 1 (-1.01430) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62065 HOMO: -6.55250 LUMO: -0.75648 factor:1 | 1 (-0.87457) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60605 HOMO: -6.81101 LUMO: -1.02043 factor:1 | 1 (-1.85998) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89694 HOMO: -6.69672 LUMO: -2.81910 factor:1 | 1 (-2.15087) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.97691 HOMO: -6.69128 LUMO: -2.58236 factor:1 | 1 (-3.23084) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.32448 HOMO: -6.73482 LUMO: -2.06807 factor:1 | 1 (-3.57841) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68591 HOMO: -7.66545 LUMO: 0.17143 factor:1 | 1 (-2.93984) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94837 HOMO: -6.87904 LUMO: -1.25172 factor:1 | 1 (-2.20230) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31185 HOMO: -6.84366 LUMO: -0.19320 factor:1 | 1 (-0.56578) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27615 HOMO: -6.97972 LUMO: -0.97961 factor:1 | 1 (-0.53008) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60576 HOMO: -6.72121 LUMO: -0.70477 factor:1 | 1 (-0.85969) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47341 HOMO: -7.18925 LUMO: 0.40001 factor:1 | 1 (-0.72733) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27838 HOMO: -6.72121 LUMO: 0.19592 factor:1 | 1 (-0.53231) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.02157 HOMO: -6.85999 LUMO: -0.39457 factor:1 | 1 (-2.27550) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29538 HOMO: -6.90625 LUMO: 0.05987 factor:1 | 1 (-1.54931) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28294 HOMO: -7.00421 LUMO: 0.37552 factor:1 | 1 (-1.53687) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63786 HOMO: -6.56883 LUMO: -0.97689 factor:1 | 1 (-1.89179) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46251 HOMO: -6.66679 LUMO: 0.56055 factor:1 | 1 (-1.71644) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.34313 HOMO: -6.75931 LUMO: 0.32926 factor:1 | 1 (-2.59705) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31382 HOMO: -6.53617 LUMO: -1.06397 factor:1 | 1 (-2.56775) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.25589 HOMO: -6.78108 LUMO: 0.42722 factor:1 | 1 (-2.50981) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60316 HOMO: -7.05319 LUMO: 0.61498 factor:1 | 1 (-2.85709) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55967 HOMO: -6.78380 LUMO: 1.49391 factor:1 | 1 (-2.81360) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89033 HOMO: -7.21102 LUMO: 0.27211 factor:1 | 1 (-2.14426) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00013 HOMO: -6.67223 LUMO: 0.81362 factor:1 | 1 (-2.25406) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80227 HOMO: -6.69944 LUMO: 1.40683 factor:1 | 1 (-2.05620) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49439 HOMO: -7.02598 LUMO: 1.46941 factor:1 | 1 (-2.74832) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.28859 HOMO: -5.85045 LUMO: -0.76736 factor:1 | 1 (-2.54252) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01759 HOMO: -6.53890 LUMO: -0.50885 factor:1 | 1 (-3.27152) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72055 HOMO: -6.42733 LUMO: -0.63947 factor:1 | 1 (-2.97448) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.58218 HOMO: -6.82189 LUMO: -0.85444 factor:1 | 1 (-2.83611) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90312 HOMO: -6.97428 LUMO: -1.22179 factor:1 | 1 (-2.15705) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.04592 HOMO: -6.93346 LUMO: -1.09934 factor:1 | 1 (-2.29985) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84943 HOMO: -7.17292 LUMO: -1.11839 factor:1 | 1 (-2.10336) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70298 HOMO: -7.00965 LUMO: -1.23268 factor:1 | 1 (-1.95691) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73171 HOMO: -6.73210 LUMO: -1.12383 factor:1 | 1 (-1.98564) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45233 HOMO: -7.61375 LUMO: -0.11973 factor:1 | 1 (-1.70626) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57310 HOMO: -7.42327 LUMO: 0.41906 factor:1 | 1 (-1.82703) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46863 HOMO: -6.94162 LUMO: -1.01771 factor:1 | 1 (-1.72256) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72129 HOMO: -6.82189 LUMO: -0.92791 factor:1 | 1 (-1.97522) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47817 HOMO: -6.92258 LUMO: -1.73881 factor:1 | 1 (-0.73210) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34701 HOMO: -6.50896 LUMO: -1.60819 factor:1 | 1 (-0.60094) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34723 HOMO: -6.38379 LUMO: -2.18780 factor:1 | 1 (-0.60115) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08345 HOMO: -6.48992 LUMO: -0.97417 factor:1 | 1 (-2.33738) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.11575 HOMO: -6.01644 LUMO: -0.04354 factor:1 | 1 (-2.36968) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45937 HOMO: -6.70761 LUMO: -0.14422 factor:1 | 1 (-2.71330) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20116 HOMO: -6.70216 LUMO: 0.14422 factor:1 | 1 (-2.45509) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47819 HOMO: -7.07224 LUMO: -0.10885 factor:1 | 1 (-1.73211) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03820 HOMO: -7.52667 LUMO: -0.74287 factor:1 | 1 (-2.29212) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32379 HOMO: -6.48447 LUMO: -0.96056 factor:1 | 1 (-1.57772) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33995 HOMO: -6.22597 LUMO: -0.41361 factor:1 | 1 (-1.59388) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03497 HOMO: -6.12256 LUMO: -1.05852 factor:1 | 1 (-1.28889) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59721 HOMO: -6.97428 LUMO: -0.60681 factor:1 | 1 (-1.85114) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71416 HOMO: -6.78380 LUMO: -0.88981 factor:1 | 1 (-1.96809) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50066 HOMO: -6.85999 LUMO: 0.07891 factor:1 | 1 (-1.75459) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15189 HOMO: -7.08312 LUMO: -0.60137 factor:1 | 1 (-1.40582) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70584 HOMO: -6.57699 LUMO: -0.68028 factor:1 | 1 (-0.95977) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66157 HOMO: -6.09807 LUMO: -0.31837 factor:1 | 1 (-0.91550) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65409 HOMO: -6.10624 LUMO: 0.14966 factor:1 | 1 (-0.90802) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.69782 HOMO: -6.77019 LUMO: -0.95784 factor:1 | 1 (-0.95175) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.84335 HOMO: -5.93208 LUMO: -0.44627 factor:1 | 1 (-0.09728) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.69915 HOMO: -6.12256 LUMO: -0.27756 factor:1 | 1 (-0.95308) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10986 HOMO: -5.98106 LUMO: -0.37824 factor:1 | 1 (-0.36379) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77333 HOMO: -7.06408 LUMO: -1.12927 factor:1 | 1 (-1.02726) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.74359 HOMO: -6.70761 LUMO: -0.98505 factor:1 | 1 (-0.99751) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89964 HOMO: -7.00965 LUMO: -0.42722 factor:1 | 1 (-1.15357) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71553 HOMO: -5.96201 LUMO: -0.59049 factor:1 | 1 (-0.96946) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.32369 HOMO: -6.34570 LUMO: -1.68438 factor:1 | 1 (-0.57762) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27014 HOMO: -6.97156 LUMO: -1.85854 factor:1 | 1 (-0.52406) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.32570 HOMO: -5.91848 LUMO: -2.51433 factor:1 | 1 (-0.57963) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43994 HOMO: -6.39195 LUMO: -1.66262 factor:1 | 1 (-0.69386) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49509 HOMO: -6.50352 LUMO: 0.19592 factor:1 | 1 (-0.74902) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37694 HOMO: -6.45998 LUMO: 0.34831 factor:1 | 1 (-0.63087) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.32510 HOMO: -7.05319 LUMO: 0.23402 factor:1 | 1 (-0.57903) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.16615 HOMO: -6.61237 LUMO: 0.18232 factor:1 | 1 (-1.42008) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50580 HOMO: -6.57427 LUMO: 0.40545 factor:1 | 1 (-1.75973) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32145 HOMO: -7.26544 LUMO: 0.41089 factor:1 | 1 (-1.57538) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18594 HOMO: -6.26406 LUMO: -0.85444 factor:1 | 1 (-1.43986) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34730 HOMO: -6.25318 LUMO: -0.79457 factor:1 | 1 (-1.60123) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41237 HOMO: -6.68040 LUMO: 0.41089 factor:1 | 1 (-0.66630) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.61695 HOMO: -6.37835 LUMO: 0.37280 factor:1 | 1 (-0.87087) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44358 HOMO: -6.56067 LUMO: 0.62858 factor:1 | 1 (-0.69751) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.61548 HOMO: -6.74026 LUMO: -0.04082 factor:1 | 1 (-0.86940) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36037 HOMO: -6.53617 LUMO: 0.35103 factor:1 | 1 (-0.61430) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35100 HOMO: -6.51985 LUMO: 0.25851 factor:1 | 1 (-1.60493) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10468 HOMO: -6.58788 LUMO: -1.98371 factor:1 | 1 (-1.35861) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49555 HOMO: -6.51441 LUMO: 0.29116 factor:1 | 1 (-1.74947) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49089 HOMO: -6.81101 LUMO: 0.35647 factor:1 | 1 (-1.74482) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39533 HOMO: -6.42733 LUMO: 0.10340 factor:1 | 1 (-1.64925) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12732 HOMO: -6.70761 LUMO: 0.28028 factor:1 | 1 (-1.38125) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47165 HOMO: -6.67495 LUMO: 0.01633 factor:1 | 1 (-1.72558) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27429 HOMO: -6.75387 LUMO: 0.15510 factor:1 | 1 (-1.52822) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07339 HOMO: -6.56067 LUMO: 0.35919 factor:1 | 1 (-1.32732) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36852 HOMO: -7.16748 LUMO: 0.21497 factor:1 | 1 (-1.62245) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.78236 HOMO: -6.71849 LUMO: 0.26667 factor:1 | 1 (-1.03629) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71869 HOMO: -6.69128 LUMO: 0.55783 factor:1 | 1 (-0.97262) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.91154 HOMO: -6.71305 LUMO: 0.45987 factor:1 | 1 (-1.16546) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76174 HOMO: -5.90487 LUMO: -0.70750 factor:1 | 1 (-1.01566) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23992 HOMO: -6.84638 LUMO: -0.72110 factor:1 | 1 (-1.49385) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40330 HOMO: -6.66135 LUMO: -1.13471 factor:1 | 1 (-1.65723) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47900 HOMO: -6.74026 LUMO: -0.64763 factor:1 | 1 (-1.73293) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29266 HOMO: -6.69672 LUMO: -1.05036 factor:1 | 1 (-1.54659) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24928 HOMO: -6.78924 LUMO: -1.03675 factor:1 | 1 (-1.50321) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.32257 HOMO: -6.81373 LUMO: -0.85988 factor:1 | 1 (-0.57650) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27378 HOMO: -7.26544 LUMO: 0.91158 factor:1 | 1 (-0.52771) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52459 HOMO: -6.64230 LUMO: -1.92929 factor:1 | 1 (-0.77852) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42298 HOMO: -7.20830 LUMO: 0.11429 factor:1 | 1 (-0.67691) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29400 HOMO: -7.17020 LUMO: 0.04898 factor:1 | 1 (-0.54793) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39014 HOMO: -7.16476 LUMO: 0.04898 factor:1 | 1 (-0.64407) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41642 HOMO: -6.59332 LUMO: -0.49253 factor:1 | 1 (-0.67035) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55955 HOMO: -7.46953 LUMO: 0.84083 factor:1 | 1 (-1.81348) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54246 HOMO: -7.39878 LUMO: 0.88709 factor:1 | 1 (-1.79639) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48942 HOMO: -6.84094 LUMO: -0.61498 factor:1 | 1 (-1.74335) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69367 HOMO: -6.03549 LUMO: -0.27211 factor:1 | 1 (-1.94760) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50317 HOMO: -7.31170 LUMO: -0.64763 factor:1 | 1 (-1.75709) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39182 HOMO: -6.88992 LUMO: -0.84627 factor:1 | 1 (-1.64574) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46763 HOMO: -7.12666 LUMO: -0.09252 factor:1 | 1 (-1.72156) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41130 HOMO: -6.70489 LUMO: -0.63675 factor:1 | 1 (-1.66523) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21505 HOMO: -6.98788 LUMO: 0.86804 factor:1 | 1 (-1.46898) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21902 HOMO: -6.80285 LUMO: -0.60954 factor:1 | 1 (-1.47295) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07165 HOMO: -7.02054 LUMO: -0.74287 factor:1 | 1 (-1.32558) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20947 HOMO: -7.03686 LUMO: -0.81090 factor:1 | 1 (-1.46340) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.05489 HOMO: -6.70489 LUMO: -1.00954 factor:1 | 1 (-1.30881) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02169 HOMO: -7.69810 LUMO: 0.00544 factor:1 | 1 (-1.27562) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04563 HOMO: -6.83550 LUMO: -0.11157 factor:1 | 1 (-1.29956) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83046 HOMO: -6.76203 LUMO: -2.13609 factor:1 | 1 (-2.08439) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83607 HOMO: -6.72121 LUMO: -2.62862 factor:1 | 1 (-2.09000) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33660 HOMO: -6.48719 LUMO: -2.73474 factor:1 | 1 (-1.59053) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46795 HOMO: -6.83006 LUMO: -0.00544 factor:1 | 1 (-1.72188) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.28655 HOMO: -6.84094 LUMO: -1.11022 factor:1 | 1 (-2.54048) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.06953 HOMO: -6.66951 LUMO: -1.23812 factor:1 | 1 (-3.32346) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.98809 HOMO: -6.78380 LUMO: -1.27894 factor:1 | 1 (-3.24202) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.81963 HOMO: -6.50352 LUMO: -0.56055 factor:1 | 1 (-3.07355) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49790 HOMO: -7.77974 LUMO: -0.26395 factor:1 | 1 (-2.75183) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.46027 HOMO: -7.01510 LUMO: -1.64085 factor:1 | 1 (-2.71420) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.07343 HOMO: -6.59876 LUMO: -0.91158 factor:1 | 1 (-2.32736) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95983 HOMO: -4.67219 LUMO: -0.67756 factor:1 | 1 (-2.21376) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.24342 HOMO: -6.70489 LUMO: -0.65579 factor:1 | 1 (-2.49735) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55329 HOMO: -6.62325 LUMO: -0.60409 factor:1 | 1 (-1.80722) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37837 HOMO: -6.20147 LUMO: 0.15238 factor:1 | 1 (-1.63230) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08906 HOMO: -6.43549 LUMO: -0.07075 factor:1 | 1 (-1.34299) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86900 HOMO: -7.02054 LUMO: 0.13061 factor:1 | 1 (-1.12293) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59079 HOMO: -7.04503 LUMO: 0.30749 factor:1 | 1 (-1.84471) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21249 HOMO: -6.74842 LUMO: -0.99594 factor:1 | 1 (-1.46642) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88715 HOMO: -6.35658 LUMO: 0.41633 factor:1 | 1 (-1.14108) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.92337 HOMO: -6.79740 LUMO: 0.56872 factor:1 | 1 (-1.17730) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46194 HOMO: -6.51713 LUMO: -0.05987 factor:1 | 1 (-1.71587) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47451 HOMO: -6.68040 LUMO: 0.34558 factor:1 | 1 (-1.72844) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21668 HOMO: -6.39740 LUMO: 0.50069 factor:1 | 1 (-1.47061) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32205 HOMO: -6.91713 LUMO: -0.97145 factor:1 | 1 (-1.57597) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27513 HOMO: -7.10761 LUMO: -0.27483 factor:1 | 1 (-1.52906) | 1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89034 HOMO: -6.98788 LUMO: 0.40273 factor:1 | 1 (-1.14427) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13263 HOMO: -6.87087 LUMO: 0.28572 factor:1 | 1 (-1.38656) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41111 HOMO: -7.36612 LUMO: -0.12245 factor:1 | 1 (-1.66504) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47481 HOMO: -6.72938 LUMO: 0.33742 factor:1 | 1 (-1.72874) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22621 HOMO: -7.32531 LUMO: 0.07619 factor:1 | 1 (-1.48014) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26139 HOMO: -6.87087 LUMO: -0.08436 factor:1 | 1 (-1.51532) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08748 HOMO: -6.67495 LUMO: 0.85988 factor:1 | 1 (-1.34141) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42335 HOMO: -6.96339 LUMO: 0.65307 factor:1 | 1 (-1.67728) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57245 HOMO: -6.58516 LUMO: -0.78641 factor:1 | 1 (-1.82637) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20311 HOMO: -6.56883 LUMO: 0.44355 factor:1 | 1 (-1.45703) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55604 HOMO: -6.68312 LUMO: 0.43538 factor:1 | 1 (-1.80997) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27528 HOMO: -6.81917 LUMO: 0.20681 factor:1 | 1 (-0.52921) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67278 HOMO: -6.91169 LUMO: 0.08163 factor:1 | 1 (-0.92671) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43305 HOMO: -4.88444 LUMO: -0.49253 factor:1 | 1 (-0.68698) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.69197 HOMO: -6.42189 LUMO: 0.64763 factor:1 | 1 (-0.94589) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36720 HOMO: -6.24501 LUMO: 0.55783 factor:1 | 1 (-0.62113) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43180 HOMO: -6.41372 LUMO: 0.29388 factor:1 | 1 (-0.68573) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.18926 HOMO: -5.67902 LUMO: 1.77690 factor:1 | 1 (-0.44319) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47191 HOMO: -6.55794 LUMO: 0.05170 factor:1 | 1 (-0.72584) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35863 HOMO: -6.52801 LUMO: 0.25851 factor:1 | 1 (-0.61256) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.12298 HOMO: -7.08857 LUMO: 0.11157 factor:1 | 1 (-0.37690) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08013 HOMO: -6.58243 LUMO: 0.75648 factor:1 | 1 (-2.33406) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21070 HOMO: -7.22190 LUMO: 0.45171 factor:1 | 1 (-1.46463) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47655 HOMO: -6.47087 LUMO: 0.00000 factor:1 | 1 (-1.73048) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36542 HOMO: -6.78652 LUMO: 1.32247 factor:1 | 1 (-1.61935) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65546 HOMO: -6.74026 LUMO: 1.45309 factor:1 | 1 (-2.90939) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.08352 HOMO: -6.69944 LUMO: 0.76464 factor:1 | 1 (-3.33745) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.07038 HOMO: -6.62325 LUMO: 0.64763 factor:1 | 1 (-3.32431) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.27681 HOMO: -6.45182 LUMO: 0.49253 factor:1 | 1 (-2.53074) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52027 HOMO: -7.14843 LUMO: 0.62586 factor:1 | 1 (-2.77420) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14768 HOMO: -6.87087 LUMO: 1.53200 factor:1 | 1 (-1.40160) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47946 HOMO: -6.54978 LUMO: 0.45171 factor:1 | 1 (-1.73339) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26077 HOMO: -6.63686 LUMO: 0.80001 factor:1 | 1 (-1.51469) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40578 HOMO: -7.00693 LUMO: 1.56193 factor:1 | 1 (-1.65970) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04882 HOMO: -6.02460 LUMO: 1.72792 factor:1 | 1 (-1.30275) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88057 HOMO: -6.36746 LUMO: -1.20002 factor:1 | 1 (-1.13450) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08250 HOMO: -7.26816 LUMO: -1.06397 factor:1 | 1 (-1.33643) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55095 HOMO: -7.34707 LUMO: -1.09662 factor:1 | 1 (-1.80488) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29277 HOMO: -7.93212 LUMO: -0.13606 factor:1 | 1 (-1.54670) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44994 HOMO: -6.80285 LUMO: 0.58504 factor:1 | 1 (-1.70387) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20809 HOMO: -7.12938 LUMO: 0.32926 factor:1 | 1 (-1.46201) | 1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00248 HOMO: -6.86815 LUMO: -1.30070 factor:1 | 1 (-1.25640) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.07368 HOMO: -6.99333 LUMO: -1.03947 factor:1 | 1 (-2.32761) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99009 HOMO: -7.56749 LUMO: -0.11157 factor:1 | 1 (-2.24401) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45989 HOMO: -7.57293 LUMO: -0.07891 factor:1 | 1 (-2.71382) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.28217 HOMO: -7.30626 LUMO: 0.27211 factor:1 | 1 (-2.53610) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37263 HOMO: -7.77974 LUMO: 0.27211 factor:1 | 1 (-1.62656) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01745 HOMO: -7.11578 LUMO: 0.19864 factor:1 | 1 (-3.27138) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30857 HOMO: -7.71171 LUMO: 0.57688 factor:1 | 1 (-2.56250) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.41864 HOMO: -7.83688 LUMO: 0.37824 factor:1 | 1 (-2.67257) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.75848 HOMO: -6.94979 LUMO: -1.66534 factor:1 | 1 (-3.01241) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.71508 HOMO: -6.97156 LUMO: -1.13199 factor:1 | 1 (-2.96901) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32754 HOMO: -6.91441 LUMO: -1.08301 factor:1 | 1 (-1.58147) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42725 HOMO: -6.71849 LUMO: -0.74831 factor:1 | 1 (-1.68117) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41688 HOMO: -7.09401 LUMO: -1.77690 factor:1 | 1 (-1.67081) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89554 HOMO: -6.97156 LUMO: -1.45037 factor:1 | 1 (-1.14946) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01105 HOMO: -7.22462 LUMO: -1.11295 factor:1 | 1 (-1.26498) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.93458 HOMO: -7.85321 LUMO: 0.16599 factor:1 | 1 (-1.18851) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07663 HOMO: -7.71987 LUMO: 0.55511 factor:1 | 1 (-1.33056) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02522 HOMO: -7.63551 LUMO: 0.14422 factor:1 | 1 (-1.27915) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21525 HOMO: -6.98788 LUMO: -0.80546 factor:1 | 1 (-0.46918) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.92131 HOMO: -6.98788 LUMO: -1.16737 factor:1 | 1 (-0.17524) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.11451 HOMO: -6.56611 LUMO: -1.60819 factor:1 | 1 (-0.36844) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.02406 HOMO: -6.95251 LUMO: 0.66396 factor:1 | 1 (-0.27799) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.74411 HOMO: -7.35252 LUMO: 0.49797 factor:1 | -1 (0.00196) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01475 HOMO: -6.90897 LUMO: -0.81090 factor:1 | 1 (-1.26868) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71444 HOMO: -7.04503 LUMO: -1.08301 factor:1 | 1 (-0.96837) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13396 HOMO: -6.92530 LUMO: -1.29526 factor:1 | 1 (-1.38789) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58614 HOMO: -6.93074 LUMO: -1.25444 factor:1 | 1 (-0.84007) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62579 HOMO: -6.73482 LUMO: -0.62042 factor:1 | 1 (-0.87972) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52932 HOMO: -7.67633 LUMO: 0.59593 factor:1 | 1 (-0.78325) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64407 HOMO: -7.39061 LUMO: -0.19320 factor:1 | 1 (-0.89800) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42698 HOMO: -7.55388 LUMO: -0.20136 factor:1 | 1 (-0.68091) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39531 HOMO: -7.14027 LUMO: -0.99866 factor:1 | 1 (-0.64924) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55830 HOMO: -6.75931 LUMO: -0.73199 factor:1 | 1 (-0.81223) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42500 HOMO: -5.45044 LUMO: -0.18776 factor:1 | 1 (-0.67892) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50334 HOMO: -6.70761 LUMO: -0.84083 factor:1 | 1 (-0.75727) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13050 HOMO: -6.05453 LUMO: -1.06669 factor:1 | 1 (-2.38442) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99719 HOMO: -6.86815 LUMO: -0.98233 factor:1 | 1 (-2.25112) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.24974 HOMO: -6.73210 LUMO: -0.95240 factor:1 | 1 (-2.50367) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.10135 HOMO: -5.89671 LUMO: -1.05036 factor:1 | 1 (-2.35528) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32523 HOMO: -7.61102 LUMO: 0.33470 factor:1 | 1 (-1.57916) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.16825 HOMO: -7.51034 LUMO: 0.23674 factor:1 | 1 (-1.42218) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20885 HOMO: -7.41510 LUMO: 0.62858 factor:1 | 1 (-1.46278) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12319 HOMO: -6.76203 LUMO: -1.72792 factor:1 | 1 (-1.37711) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37271 HOMO: -6.60420 LUMO: -0.45715 factor:1 | 1 (-1.62664) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.87475 HOMO: -6.59060 LUMO: -0.58232 factor:1 | 1 (-0.12868) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.59622 HOMO: -7.43687 LUMO: -0.76736 factor:1 | -1 (0.14985) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.48609 HOMO: -6.08719 LUMO: -0.48708 factor:1 | -1 (0.25998) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.11441 HOMO: -5.88854 LUMO: -0.05714 factor:1 | 1 (-0.36833) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.00055 HOMO: -7.34435 LUMO: -0.71838 factor:1 | 1 (-0.25448) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.00531 HOMO: -7.46408 LUMO: -0.63130 factor:1 | 1 (-0.25924) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.78009 HOMO: -7.00965 LUMO: -1.24900 factor:1 | -1 (0.96598) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.87865 HOMO: -6.91169 LUMO: -0.88981 factor:1 | -1 (0.86742) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.89846 HOMO: -6.78652 LUMO: -0.82178 factor:1 | -1 (0.84761) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.56134 HOMO: -7.80423 LUMO: 0.87076 factor:1 | -1 (1.18473) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.97966 HOMO: -6.97700 LUMO: -1.00954 factor:1 | -1 (0.76641) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.45344 HOMO: -6.92530 LUMO: -0.88165 factor:1 | -1 (0.29263) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.06753 HOMO: -7.14571 LUMO: -1.04492 factor:1 | -1 (0.67854) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.86360 HOMO: -7.49674 LUMO: 0.34558 factor:1 | 1 (-0.11753) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21767 HOMO: -6.44094 LUMO: -1.20819 factor:1 | 1 (-0.47160) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.14015 HOMO: -6.47359 LUMO: -1.14016 factor:1 | 1 (-0.39408) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.13106 HOMO: -6.61237 LUMO: -0.87076 factor:1 | 1 (-0.38499) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.21624 HOMO: -6.73754 LUMO: -1.09662 factor:1 | 1 (-2.47017) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81027 HOMO: -6.97700 LUMO: 0.13061 factor:1 | 1 (-2.06420) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12840 HOMO: -6.82734 LUMO: 0.59865 factor:1 | 1 (-2.38233) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.96051 HOMO: -6.86543 LUMO: -0.91430 factor:1 | 1 (-2.21444) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02781 HOMO: -6.74298 LUMO: 0.28028 factor:1 | 1 (-1.28174) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32148 HOMO: -6.75387 LUMO: 0.19592 factor:1 | 1 (-1.57540) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04397 HOMO: -7.05591 LUMO: 0.10612 factor:1 | 1 (-1.29790) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27769 HOMO: -6.86543 LUMO: 0.49253 factor:1 | 1 (-1.53162) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06797 HOMO: -6.11440 LUMO: -1.12655 factor:1 | 1 (-1.32190) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03442 HOMO: -6.77291 LUMO: -1.02859 factor:1 | 1 (-1.28835) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06618 HOMO: -6.54978 LUMO: 0.29116 factor:1 | 1 (-1.32011) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07176 HOMO: -7.18108 LUMO: 0.00000 factor:1 | 1 (-1.32568) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.05309 HOMO: -6.86271 LUMO: -1.15376 factor:1 | 1 (-1.30702) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14351 HOMO: -6.78108 LUMO: -1.22723 factor:1 | 1 (-1.39744) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07227 HOMO: -6.40828 LUMO: 0.02449 factor:1 | 1 (-1.32620) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.95222 HOMO: -6.43821 LUMO: 0.09796 factor:1 | 1 (-1.20614) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.92985 HOMO: -6.99877 LUMO: 0.40545 factor:1 | 1 (-1.18378) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11584 HOMO: -6.68856 LUMO: 0.19320 factor:1 | 1 (-1.36977) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06068 HOMO: -7.11034 LUMO: 0.31293 factor:1 | 1 (-1.31461) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58625 HOMO: -6.92530 LUMO: -0.85444 factor:1 | 1 (-0.84018) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59909 HOMO: -6.60148 LUMO: -0.59865 factor:1 | 1 (-0.85302) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04577 HOMO: -6.72938 LUMO: 0.30749 factor:1 | 1 (-1.29970) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06117 HOMO: -7.31170 LUMO: 0.06803 factor:1 | 1 (-1.31510) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08572 HOMO: -7.09129 LUMO: -0.04626 factor:1 | 1 (-1.33964) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89962 HOMO: -6.38379 LUMO: -0.76736 factor:1 | 1 (-1.15355) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.93872 HOMO: -6.13617 LUMO: -0.63947 factor:1 | 1 (-1.19265) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58796 HOMO: -6.92258 LUMO: 0.37007 factor:1 | 1 (-0.84189) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86503 HOMO: -6.35930 LUMO: 0.41361 factor:1 | 1 (-1.11896) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67882 HOMO: -6.60420 LUMO: 0.26667 factor:1 | 1 (-0.93275) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02482 HOMO: -6.04909 LUMO: 1.82588 factor:1 | 1 (-1.27874) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15442 HOMO: -6.69672 LUMO: 1.72520 factor:1 | 1 (-1.40835) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87076 HOMO: -6.50080 LUMO: 0.29116 factor:1 | 1 (-2.12469) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67620 HOMO: -6.60692 LUMO: -0.43266 factor:1 | 1 (-1.93013) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66736 HOMO: -6.93890 LUMO: 0.39729 factor:1 | 1 (-1.92129) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60733 HOMO: -6.52801 LUMO: -0.47076 factor:1 | 1 (-1.86126) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70804 HOMO: -6.41100 LUMO: 0.30477 factor:1 | 1 (-1.96197) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72461 HOMO: -6.37291 LUMO: -0.80001 factor:1 | 1 (-1.97854) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86185 HOMO: -6.51985 LUMO: 1.44765 factor:1 | 1 (-1.11578) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53414 HOMO: -6.64774 LUMO: 0.04626 factor:1 | 1 (-0.78807) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42021 HOMO: -6.65863 LUMO: 0.29933 factor:1 | 1 (-0.67413) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.87807 HOMO: -7.09673 LUMO: 0.28300 factor:1 | 1 (-1.13199) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77017 HOMO: -6.57155 LUMO: -1.11567 factor:1 | 1 (-1.02410) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90394 HOMO: -6.38379 LUMO: -0.60681 factor:1 | 1 (-1.15787) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88114 HOMO: -6.60148 LUMO: 0.18232 factor:1 | 1 (-1.13507) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84879 HOMO: -6.96067 LUMO: -0.52246 factor:1 | 1 (-1.10271) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84027 HOMO: -6.57427 LUMO: -0.84627 factor:1 | 1 (-1.09420) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75131 HOMO: -6.59332 LUMO: -0.98233 factor:1 | 1 (-1.00524) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77975 HOMO: -6.20692 LUMO: -0.27483 factor:1 | 1 (-1.03368) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.25551 HOMO: -6.81373 LUMO: 0.74559 factor:1 | 1 (-2.50943) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.34247 HOMO: -6.60420 LUMO: 0.54695 factor:1 | 1 (-2.59640) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.21393 HOMO: -6.58788 LUMO: -0.31021 factor:1 | 1 (-2.46786) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08478 HOMO: -6.72938 LUMO: 0.64763 factor:1 | 1 (-2.33871) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41122 HOMO: -6.86815 LUMO: 0.32109 factor:1 | 1 (-1.66515) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42629 HOMO: -6.63141 LUMO: 0.18776 factor:1 | 1 (-1.68022) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29639 HOMO: -7.18653 LUMO: 0.09524 factor:1 | 1 (-1.55031) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46472 HOMO: -6.83550 LUMO: 0.03537 factor:1 | 1 (-1.71864) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.23746 HOMO: -7.47769 LUMO: 0.40817 factor:1 | 1 (-2.49139) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.28922 HOMO: -6.57971 LUMO: -0.63675 factor:1 | 1 (-2.54315) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.18448 HOMO: -6.74842 LUMO: -0.16327 factor:1 | 1 (-2.43841) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.21412 HOMO: -7.07224 LUMO: 0.61770 factor:1 | 1 (-2.46805) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.17126 HOMO: -6.83006 LUMO: 0.54695 factor:1 | 1 (-2.42519) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.07080 HOMO: -6.60148 LUMO: 1.23540 factor:1 | 1 (-2.32472) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54954 HOMO: -6.99061 LUMO: 0.41089 factor:1 | 1 (-0.80347) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41966 HOMO: -6.63686 LUMO: 0.85172 factor:1 | 1 (-0.67359) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35444 HOMO: -6.50624 LUMO: 0.12517 factor:1 | 1 (-0.60836) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42293 HOMO: -6.35658 LUMO: 0.36463 factor:1 | 1 (-0.67686) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91721 HOMO: -6.34570 LUMO: 0.65035 factor:1 | 1 (-2.17114) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.05488 HOMO: -6.63141 LUMO: 1.25717 factor:1 | 1 (-2.30880) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.18353 HOMO: -6.91441 LUMO: 1.32792 factor:1 | 1 (-2.43746) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03700 HOMO: -7.15387 LUMO: 0.64219 factor:1 | 1 (-2.29093) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95311 HOMO: -7.17836 LUMO: 0.60409 factor:1 | 1 (-2.20703) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75514 HOMO: -6.92258 LUMO: 0.49525 factor:1 | 1 (-2.00907) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.09980 HOMO: -6.31032 LUMO: 0.48708 factor:1 | 1 (-2.35373) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20827 HOMO: -6.49808 LUMO: 0.31021 factor:1 | 1 (-2.46220) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86826 HOMO: -6.48447 LUMO: 0.37552 factor:1 | 1 (-2.12219) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.11101 HOMO: -6.66135 LUMO: -1.08301 factor:1 | 1 (-2.36494) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03860 HOMO: -6.33481 LUMO: -0.51974 factor:1 | 1 (-2.29253) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92628 HOMO: -6.76475 LUMO: -0.15238 factor:1 | 1 (-2.18020) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99689 HOMO: -6.93346 LUMO: -0.10885 factor:1 | 1 (-2.25082) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89532 HOMO: -7.19741 LUMO: 0.73199 factor:1 | 1 (-1.14925) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04199 HOMO: -6.82734 LUMO: 0.88437 factor:1 | 1 (-1.29592) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11222 HOMO: -7.01237 LUMO: 0.02721 factor:1 | 1 (-1.36615) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.05557 HOMO: -6.39195 LUMO: 1.46941 factor:1 | 1 (-1.30949) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08255 HOMO: -6.53890 LUMO: 1.32792 factor:1 | 1 (-2.33648) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.28772 HOMO: -6.82734 LUMO: 1.98099 factor:1 | 1 (-2.54165) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.25009 HOMO: -6.74570 LUMO: 1.68983 factor:1 | 1 (-2.50402) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93836 HOMO: -6.41100 LUMO: 1.39050 factor:1 | 1 (-2.19229) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.01689 HOMO: -5.92664 LUMO: 1.65989 factor:1 | 1 (-2.27082) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97795 HOMO: -6.07630 LUMO: 1.54833 factor:1 | 1 (-2.23188) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90818 HOMO: -6.45998 LUMO: 0.68573 factor:1 | 1 (-2.16211) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86393 HOMO: -6.52801 LUMO: 0.41361 factor:1 | 1 (-2.11786) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.06211 HOMO: -6.77564 LUMO: 0.42178 factor:1 | 1 (-2.31604) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68750 HOMO: -6.56339 LUMO: 1.65717 factor:1 | 1 (-1.94142) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54812 HOMO: -5.85861 LUMO: 1.90752 factor:1 | 1 (-1.80205) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76763 HOMO: -6.77019 LUMO: -2.48440 factor:1 | 1 (-2.02156) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65258 HOMO: -6.53890 LUMO: -1.82588 factor:1 | 1 (-1.90651) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61100 HOMO: -6.50352 LUMO: -1.66806 factor:1 | 1 (-1.86493) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72050 HOMO: -6.90625 LUMO: 0.43538 factor:1 | 1 (-1.97443) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72546 HOMO: -6.85455 LUMO: 0.53062 factor:1 | 1 (-1.97938) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72102 HOMO: -6.49536 LUMO: 0.31021 factor:1 | 1 (-1.97495) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47949 HOMO: -4.97696 LUMO: -0.09252 factor:1 | 1 (-1.73342) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40651 HOMO: -5.31166 LUMO: 0.34286 factor:1 | 1 (-1.66044) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.16417 HOMO: -6.42461 LUMO: 0.74287 factor:1 | 1 (-1.41809) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23674 HOMO: -6.59604 LUMO: 0.62858 factor:1 | 1 (-1.49067) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22515 HOMO: -6.45998 LUMO: -0.61770 factor:1 | 1 (-1.47907) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06939 HOMO: -6.75659 LUMO: -0.34014 factor:1 | 1 (-1.32332) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25734 HOMO: -6.63958 LUMO: 0.36191 factor:1 | 1 (-1.51127) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30583 HOMO: -5.92936 LUMO: -0.67484 factor:1 | 1 (-1.55976) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27946 HOMO: -5.67630 LUMO: 1.80956 factor:1 | 1 (-1.53339) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21546 HOMO: -6.50352 LUMO: -0.78369 factor:1 | 1 (-1.46939) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13051 HOMO: -6.35930 LUMO: -0.75648 factor:1 | 1 (-1.38443) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19459 HOMO: -6.74298 LUMO: 0.48980 factor:1 | 1 (-1.44852) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23902 HOMO: -6.85183 LUMO: 0.15510 factor:1 | 1 (-1.49295) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03856 HOMO: -6.90897 LUMO: 0.26123 factor:1 | 1 (-1.29249) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23829 HOMO: -6.85999 LUMO: 0.47892 factor:1 | 1 (-1.49222) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96751 HOMO: -6.69944 LUMO: 0.57416 factor:1 | 1 (-1.22144) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37149 HOMO: -6.74026 LUMO: 0.69933 factor:1 | 1 (-1.62542) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08348 HOMO: -6.52801 LUMO: 0.75376 factor:1 | 1 (-1.33741) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26651 HOMO: -7.05863 LUMO: 0.44627 factor:1 | 1 (-1.52044) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10890 HOMO: -6.96339 LUMO: 0.48164 factor:1 | 1 (-1.36283) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10648 HOMO: -6.95795 LUMO: 0.44355 factor:1 | 1 (-1.36041) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02732 HOMO: -6.36746 LUMO: 0.58777 factor:1 | 1 (-1.28125) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00027 HOMO: -6.69400 LUMO: 0.40545 factor:1 | 1 (-1.25420) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.97227 HOMO: -6.30760 LUMO: -0.66668 factor:1 | 1 (-1.22620) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02310 HOMO: -6.53617 LUMO: -0.64491 factor:1 | 1 (-1.27703) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10278 HOMO: -6.80829 LUMO: 0.17415 factor:1 | 1 (-1.35671) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08280 HOMO: -6.80285 LUMO: 0.73471 factor:1 | 1 (-1.33673) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98470 HOMO: -6.43821 LUMO: 0.21769 factor:1 | 1 (-2.23863) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.23763 HOMO: -6.98788 LUMO: 0.10885 factor:1 | 1 (-2.49156) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.09346 HOMO: -7.15115 LUMO: 0.40817 factor:1 | 1 (-2.34739) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.06812 HOMO: -6.00011 LUMO: -0.98505 factor:1 | 1 (-3.32205) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.88128 HOMO: -6.16882 LUMO: -0.77825 factor:1 | 1 (-4.13521) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.16932 HOMO: -6.30760 LUMO: 0.34831 factor:1 | 1 (-3.42325) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.88412 HOMO: -6.64502 LUMO: 0.63403 factor:1 | 1 (-3.13804) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.14396 HOMO: -6.93618 LUMO: 0.96600 factor:1 | 1 (-3.39789) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45533 HOMO: -6.45182 LUMO: 0.16327 factor:1 | 1 (-1.70926) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80573 HOMO: -6.99605 LUMO: 0.20953 factor:1 | 1 (-2.05966) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59321 HOMO: -6.72665 LUMO: 0.32654 factor:1 | 1 (-1.84714) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92423 HOMO: -6.38379 LUMO: 0.45443 factor:1 | 1 (-2.17816) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99185 HOMO: -6.65318 LUMO: 0.04354 factor:1 | 1 (-2.24578) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78415 HOMO: -6.94707 LUMO: -1.68438 factor:1 | 1 (-2.03808) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54798 HOMO: -6.71849 LUMO: 0.15783 factor:1 | 1 (-1.80191) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60754 HOMO: -6.97156 LUMO: 0.43266 factor:1 | 1 (-2.86147) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.46528 HOMO: -6.91441 LUMO: -0.54695 factor:1 | 1 (-2.71921) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30057 HOMO: -6.74842 LUMO: -0.76192 factor:1 | 1 (-2.55450) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54814 HOMO: -6.70489 LUMO: 0.19048 factor:1 | 1 (-2.80207) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56512 HOMO: -7.25728 LUMO: 0.33470 factor:1 | 1 (-2.81905) | 1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.34827 HOMO: -6.96339 LUMO: 0.55511 factor:1 | 1 (-2.60220) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.80450 HOMO: -6.77564 LUMO: 0.72382 factor:1 | 1 (-3.05842) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.71100 HOMO: -6.75387 LUMO: 0.39729 factor:1 | 1 (-2.96493) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.00167 HOMO: -7.00149 LUMO: 0.06531 factor:1 | 1 (-3.25560) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.02361 HOMO: -7.09945 LUMO: 0.33470 factor:1 | 1 (-2.27754) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14394 HOMO: -7.20830 LUMO: 0.59593 factor:1 | 1 (-2.39787) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30343 HOMO: -6.40556 LUMO: 0.56600 factor:1 | 1 (-2.55735) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.17961 HOMO: -6.77291 LUMO: 0.73471 factor:1 | 1 (-2.43354) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.03245 HOMO: -6.65046 LUMO: 0.09796 factor:1 | 1 (-3.28637) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.80993 HOMO: -6.95795 LUMO: 0.22313 factor:1 | 1 (-4.06386) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.20056 HOMO: -6.85727 LUMO: 0.04626 factor:1 | 1 (-3.45449) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01503 HOMO: -7.27360 LUMO: 0.42178 factor:1 | 1 (-3.26896) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.24758 HOMO: -6.78924 LUMO: -0.13334 factor:1 | 1 (-3.50151) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99615 HOMO: -6.63141 LUMO: 0.38368 factor:1 | 1 (-2.25008) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.90771 HOMO: -6.92258 LUMO: 0.39184 factor:1 | 1 (-3.16164) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.04780 HOMO: -6.19331 LUMO: -0.46804 factor:1 | 1 (-2.30173) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.02595 HOMO: -7.26544 LUMO: -0.05442 factor:1 | 1 (-2.27988) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88377 HOMO: -7.09401 LUMO: 0.30749 factor:1 | 1 (-2.13770) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81257 HOMO: -6.14705 LUMO: -0.88709 factor:1 | 1 (-1.06650) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65088 HOMO: -6.53617 LUMO: -0.28572 factor:1 | 1 (-0.90481) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81200 HOMO: -6.37291 LUMO: -0.67212 factor:1 | 1 (-1.06592) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.87096 HOMO: -6.65591 LUMO: 0.03810 factor:1 | 1 (-1.12489) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60050 HOMO: -7.11034 LUMO: 0.75103 factor:1 | 1 (-1.85443) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41190 HOMO: -6.85183 LUMO: -0.05987 factor:1 | 1 (-1.66583) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00015 HOMO: -6.70761 LUMO: -0.05442 factor:1 | 1 (-2.25408) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90698 HOMO: -6.23413 LUMO: 0.06259 factor:1 | 1 (-2.16091) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00443 HOMO: -6.55794 LUMO: 0.74015 factor:1 | 1 (-2.25835) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63356 HOMO: -7.27905 LUMO: 0.26939 factor:1 | 1 (-1.88749) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56281 HOMO: -6.34842 LUMO: -0.86804 factor:1 | 1 (-1.81674) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75522 HOMO: -6.27222 LUMO: 1.46125 factor:1 | 1 (-2.00915) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.62065 HOMO: -6.65046 LUMO: 2.04902 factor:1 | -1 (0.12542) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.71734 HOMO: -7.11850 LUMO: -1.14016 factor:1 | -1 (0.02874) | 1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50693 HOMO: -6.88720 LUMO: -1.20274 factor:1 | 1 (-0.76086) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.07136 HOMO: -6.69400 LUMO: -0.31565 factor:1 | 1 (-0.32528) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.37024 HOMO: -6.95523 LUMO: -1.55377 factor:1 | -1 (1.37583) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.77882 HOMO: -6.41372 LUMO: -0.83539 factor:1 | -1 (0.96726) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.62529 HOMO: -6.13889 LUMO: -0.90070 factor:1 | -1 (1.12078) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.34395 HOMO: -6.44366 LUMO: -0.55511 factor:1 | -1 (1.40212) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.29455 HOMO: -6.10079 LUMO: -0.71022 factor:1 | -1 (0.45152) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.05422 HOMO: -6.90353 LUMO: -0.64763 factor:1 | -1 (0.69185) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.00241 HOMO: -6.65046 LUMO: -0.82450 factor:1 | -1 (0.74366) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.70532 HOMO: -6.81645 LUMO: -0.85444 factor:1 | -1 (1.04075) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46279 HOMO: -6.20692 LUMO: 1.30887 factor:1 | 1 (-0.71672) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41354 HOMO: -5.96201 LUMO: 1.33880 factor:1 | 1 (-0.66747) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.57569 HOMO: -6.52529 LUMO: 1.58914 factor:1 | 1 (-0.82962) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56152 HOMO: -6.58516 LUMO: 1.97555 factor:1 | 1 (-0.81544) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35084 HOMO: -6.84366 LUMO: 0.15783 factor:1 | 1 (-0.60477) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50287 HOMO: -6.45726 LUMO: 0.42994 factor:1 | 1 (-0.75680) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53373 HOMO: -6.75387 LUMO: 0.14422 factor:1 | 1 (-0.78766) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59126 HOMO: -6.69944 LUMO: 1.79051 factor:1 | 1 (-0.84519) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30749 HOMO: -6.59876 LUMO: 1.90208 factor:1 | 1 (-1.56142) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55577 HOMO: -7.05863 LUMO: 1.20819 factor:1 | 1 (-1.80969) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65557 HOMO: -6.54978 LUMO: 2.01636 factor:1 | 1 (-2.90950) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52288 HOMO: -5.52119 LUMO: 1.95106 factor:1 | 1 (-2.77681) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.18173 HOMO: -6.53617 LUMO: 1.60275 factor:1 | 1 (-3.43566) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.37777 HOMO: -6.11440 LUMO: 1.89119 factor:1 | 1 (-2.63169) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62773 HOMO: -7.31986 LUMO: 0.48708 factor:1 | 1 (-2.88166) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50080 HOMO: -6.76475 LUMO: -0.75648 factor:1 | 1 (-1.75473) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53707 HOMO: -6.76747 LUMO: -1.06941 factor:1 | 1 (-1.79100) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47582 HOMO: -6.87087 LUMO: 0.72927 factor:1 | 1 (-1.72975) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54491 HOMO: -7.00965 LUMO: 0.02177 factor:1 | 1 (-1.79884) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63055 HOMO: -6.54706 LUMO: -0.03265 factor:1 | 1 (-0.88448) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54288 HOMO: -6.62325 LUMO: -0.63675 factor:1 | 1 (-0.79680) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43392 HOMO: -7.03414 LUMO: -1.24084 factor:1 | 1 (-0.68785) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65058 HOMO: -7.04503 LUMO: -0.10068 factor:1 | 1 (-0.90451) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52527 HOMO: -6.67223 LUMO: 0.03537 factor:1 | 1 (-0.77920) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44529 HOMO: -6.82734 LUMO: 0.58777 factor:1 | 1 (-1.69922) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23271 HOMO: -6.84366 LUMO: 0.46531 factor:1 | 1 (-1.48664) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26319 HOMO: -7.03959 LUMO: -1.15104 factor:1 | 1 (-1.51712) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47489 HOMO: -6.91169 LUMO: -0.41361 factor:1 | 1 (-1.72882) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28518 HOMO: -7.10217 LUMO: -0.44627 factor:1 | 1 (-1.53910) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73333 HOMO: -6.88176 LUMO: -0.19592 factor:1 | 1 (-0.98726) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84217 HOMO: -7.21374 LUMO: -0.46531 factor:1 | 1 (-1.09610) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90841 HOMO: -6.54978 LUMO: 0.16871 factor:1 | 1 (-1.16233) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.94503 HOMO: -6.71305 LUMO: -0.13061 factor:1 | 1 (-1.19896) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27865 HOMO: -6.74842 LUMO: -0.36191 factor:1 | 1 (-0.53258) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10186 HOMO: -6.74570 LUMO: -0.09796 factor:1 | 1 (-0.35579) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.22883 HOMO: -6.93890 LUMO: -0.27211 factor:1 | 1 (-0.48276) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38538 HOMO: -6.88720 LUMO: -0.18776 factor:1 | 1 (-0.63930) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34644 HOMO: -6.74842 LUMO: 0.02993 factor:1 | 1 (-0.60036) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33367 HOMO: -6.70216 LUMO: 0.01361 factor:1 | 1 (-0.58760) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31988 HOMO: -6.90625 LUMO: 0.00544 factor:1 | 1 (-0.57381) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52420 HOMO: -6.18243 LUMO: 0.25851 factor:1 | 1 (-1.77813) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59343 HOMO: -6.32937 LUMO: -0.20953 factor:1 | 1 (-1.84735) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28776 HOMO: -6.78108 LUMO: 0.00544 factor:1 | 1 (-1.54169) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42953 HOMO: -5.97562 LUMO: 0.28572 factor:1 | 1 (-1.68346) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.12398 HOMO: -5.97290 LUMO: -0.18504 factor:1 | 1 (-0.37791) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.00602 HOMO: -6.12800 LUMO: 0.42178 factor:1 | 1 (-0.25995) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.24799 HOMO: -6.24229 LUMO: -0.00816 factor:1 | 1 (-0.50191) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.13002 HOMO: -6.61781 LUMO: 0.12789 factor:1 | 1 (-0.38395) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48557 HOMO: -6.70489 LUMO: 0.14694 factor:1 | 1 (-0.73950) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29210 HOMO: -6.86543 LUMO: -0.21225 factor:1 | 1 (-0.54602) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.16412 HOMO: -6.90081 LUMO: -0.20136 factor:1 | 1 (-0.41805) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.08589 HOMO: -7.12938 LUMO: -0.25851 factor:1 | 1 (-0.33982) | 1 | 1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17797 HOMO: -6.93074 LUMO: -0.26667 factor:1 | 1 (-0.43190) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27071 HOMO: -7.00421 LUMO: -0.31021 factor:1 | 1 (-0.52464) | -1 | -1 |
| G: -5245.38038 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.06322 HOMO: -7.10761 LUMO: -0.17415 factor:1 | 1 (-0.31715) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95145 HOMO: -8.21240 LUMO: 0.05987 factor:1 | 1 (-2.20537) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13080 HOMO: -7.14843 LUMO: -0.46531 factor:1 | 1 (-1.38473) | 1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23764 HOMO: -6.80829 LUMO: -0.29933 factor:1 | 1 (-1.49156) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31562 HOMO: -6.84094 LUMO: -0.53606 factor:1 | 1 (-1.56955) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60349 HOMO: -6.81917 LUMO: -0.26667 factor:1 | 1 (-1.85742) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78429 HOMO: -6.85727 LUMO: -1.20002 factor:1 | 1 (-2.03821) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68945 HOMO: -6.39468 LUMO: -1.06941 factor:1 | 1 (-2.94337) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.44396 HOMO: -6.00827 LUMO: -1.94017 factor:1 | 1 (-3.69789) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.32606 HOMO: -6.80829 LUMO: 0.18504 factor:1 | 1 (-3.57998) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.59230 HOMO: -6.54434 LUMO: -0.95784 factor:1 | 1 (-2.84623) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68131 HOMO: -6.45454 LUMO: -0.07347 factor:1 | 1 (-2.93524) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35938 HOMO: -5.33887 LUMO: 1.11839 factor:1 | 1 (-1.61331) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40031 HOMO: -5.75249 LUMO: 0.70477 factor:1 | 1 (-1.65423) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22550 HOMO: -5.64092 LUMO: 0.87076 factor:1 | 1 (-1.47943) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48994 HOMO: -5.14295 LUMO: 1.06124 factor:1 | 1 (-1.74387) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21127 HOMO: -5.05043 LUMO: 1.21091 factor:1 | 1 (-1.46520) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34150 HOMO: -5.05588 LUMO: 1.02859 factor:1 | 1 (-1.59543) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53259 HOMO: -5.76337 LUMO: 0.79457 factor:1 | 1 (-0.78652) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62456 HOMO: -5.01506 LUMO: 1.00138 factor:1 | 1 (-0.87849) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53776 HOMO: -4.84363 LUMO: 1.53744 factor:1 | 1 (-0.79169) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.74598 HOMO: -5.17833 LUMO: 1.45309 factor:1 | 1 (-0.99991) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66024 HOMO: -5.13751 LUMO: 0.51157 factor:1 | 1 (-0.91417) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56309 HOMO: -5.56473 LUMO: 0.32109 factor:1 | 1 (-0.81702) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39633 HOMO: -4.69941 LUMO: 1.14016 factor:1 | 1 (-1.65026) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40123 HOMO: -4.49260 LUMO: 1.86398 factor:1 | 1 (-1.65516) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56398 HOMO: -4.32117 LUMO: 1.68438 factor:1 | 1 (-1.81791) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52733 HOMO: -4.44906 LUMO: 1.37690 factor:1 | 1 (-1.78126) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76116 HOMO: -4.62049 LUMO: 1.34968 factor:1 | 1 (-2.01508) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.21340 HOMO: -4.59600 LUMO: 1.58370 factor:1 | 1 (-3.46733) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.43945 HOMO: -4.98785 LUMO: 1.46669 factor:1 | 1 (-2.69338) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.59434 HOMO: -5.06676 LUMO: 1.27349 factor:1 | 1 (-2.84827) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54155 HOMO: -5.09125 LUMO: 1.13471 factor:1 | 1 (-2.79548) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68564 HOMO: -4.84635 LUMO: 1.33608 factor:1 | 1 (-2.93956) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61381 HOMO: -4.94431 LUMO: 1.18370 factor:1 | 1 (-1.86774) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80170 HOMO: -4.92526 LUMO: 1.39867 factor:1 | 1 (-2.05563) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92908 HOMO: -5.71983 LUMO: 0.60137 factor:1 | 1 (-2.18301) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70889 HOMO: -5.10486 LUMO: 1.05580 factor:1 | 1 (-0.96282) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54162 HOMO: -5.20282 LUMO: 1.01226 factor:1 | 1 (-0.79555) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89306 HOMO: -4.98513 LUMO: 1.53744 factor:1 | 1 (-1.14699) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99039 HOMO: -5.67085 LUMO: 0.17687 factor:1 | 1 (-1.24432) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20689 HOMO: -5.87222 LUMO: 0.12517 factor:1 | 1 (-1.46082) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17862 HOMO: -5.20826 LUMO: 0.91702 factor:1 | 1 (-1.43254) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.05788 HOMO: -5.94569 LUMO: 0.63130 factor:1 | 1 (-1.31181) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25312 HOMO: -5.35792 LUMO: 0.91430 factor:1 | 1 (-1.50705) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29647 HOMO: -5.36336 LUMO: 1.44220 factor:1 | 1 (-1.55040) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84546 HOMO: -5.83412 LUMO: 0.71294 factor:1 | 1 (-2.09939) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54828 HOMO: -4.97696 LUMO: 1.72792 factor:1 | 1 (-1.80221) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20459 HOMO: -5.55929 LUMO: 0.23130 factor:1 | 1 (-2.45852) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82763 HOMO: -5.71167 LUMO: 0.47348 factor:1 | 1 (-2.08156) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54534 HOMO: -7.31986 LUMO: -2.54699 factor:1 | 1 (-1.79927) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50643 HOMO: -5.34704 LUMO: 1.19730 factor:1 | 1 (-1.76036) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61767 HOMO: -5.45860 LUMO: 0.80818 factor:1 | 1 (-1.87160) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87934 HOMO: -5.12663 LUMO: 1.20274 factor:1 | 1 (-2.13326) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58328 HOMO: -5.37153 LUMO: 1.05580 factor:1 | 1 (-1.83720) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64189 HOMO: -5.47221 LUMO: 0.97961 factor:1 | 1 (-1.89582) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38412 HOMO: -5.06948 LUMO: 1.12111 factor:1 | 1 (-1.63804) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48175 HOMO: -5.19737 LUMO: 1.25444 factor:1 | 1 (-1.73568) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74905 HOMO: -5.27901 LUMO: 1.00682 factor:1 | 1 (-2.00298) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65694 HOMO: -5.38513 LUMO: 0.49253 factor:1 | 1 (-1.91087) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.16251 HOMO: -5.12390 LUMO: 1.22995 factor:1 | 1 (-1.41643) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12125 HOMO: -5.31438 LUMO: 0.70205 factor:1 | 1 (-1.37518) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09021 HOMO: -5.17561 LUMO: 1.04492 factor:1 | 1 (-1.34413) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14169 HOMO: -4.94431 LUMO: 1.52656 factor:1 | 1 (-1.39562) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17432 HOMO: -5.13751 LUMO: 0.93879 factor:1 | 1 (-1.42824) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96291 HOMO: -5.49942 LUMO: 0.97689 factor:1 | 1 (-1.21684) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23500 HOMO: -5.79058 LUMO: 0.53879 factor:1 | 1 (-1.48893) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99975 HOMO: -5.36881 LUMO: 1.56465 factor:1 | 1 (-2.25367) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.09700 HOMO: -4.67492 LUMO: 1.32792 factor:1 | 1 (-2.35093) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84519 HOMO: -4.60145 LUMO: 1.19458 factor:1 | 1 (-2.09911) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03694 HOMO: -4.49260 LUMO: 1.60547 factor:1 | 1 (-2.29087) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03787 HOMO: -4.65043 LUMO: 1.34696 factor:1 | 1 (-2.29180) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46436 HOMO: -4.77560 LUMO: 1.35241 factor:1 | 1 (-1.71829) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67914 HOMO: -4.94431 LUMO: 1.17825 factor:1 | 1 (-1.93307) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61756 HOMO: -4.87084 LUMO: 1.41771 factor:1 | 1 (-1.87149) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57272 HOMO: -5.34432 LUMO: 1.16737 factor:1 | 1 (-1.82665) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65737 HOMO: -4.94975 LUMO: 1.67622 factor:1 | 1 (-1.91130) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63457 HOMO: -4.81369 LUMO: 1.14288 factor:1 | 1 (-1.88850) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57283 HOMO: -5.22459 LUMO: 0.29660 factor:1 | 1 (-1.82675) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79591 HOMO: -5.21642 LUMO: 0.37824 factor:1 | 1 (-2.04983) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08486 HOMO: -5.00417 LUMO: 1.01226 factor:1 | 1 (-2.33879) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70028 HOMO: -5.46677 LUMO: 0.10612 factor:1 | 1 (-1.95421) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89411 HOMO: -5.51303 LUMO: 0.54151 factor:1 | 1 (-2.14804) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82875 HOMO: -5.63004 LUMO: 0.17960 factor:1 | 1 (-2.08268) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93746 HOMO: -4.79193 LUMO: 1.12111 factor:1 | 1 (-2.19139) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91210 HOMO: -5.43411 LUMO: 0.45987 factor:1 | 1 (-2.16603) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.59053 HOMO: -7.06135 LUMO: -2.13881 factor:1 | -1 (0.15554) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.74901 HOMO: -5.33071 LUMO: 1.14016 factor:1 | 1 (-0.00294) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.73614 HOMO: -7.12394 LUMO: -0.03810 factor:1 | -1 (0.00993) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.03737 HOMO: -7.20558 LUMO: -2.50889 factor:1 | 1 (-0.29130) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.90480 HOMO: -7.26816 LUMO: -2.11432 factor:1 | 1 (-0.15872) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.82983 HOMO: -7.89674 LUMO: 0.31021 factor:1 | 1 (-0.08376) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.96698 HOMO: -7.26544 LUMO: 0.22858 factor:1 | 1 (-2.22091) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.28538 HOMO: -7.12666 LUMO: -0.02449 factor:1 | 1 (-2.53931) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.17969 HOMO: -7.68722 LUMO: 0.71838 factor:1 | 1 (-2.43362) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01771 HOMO: -6.86271 LUMO: -0.96056 factor:1 | 1 (-1.27164) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89154 HOMO: -7.07496 LUMO: -1.11839 factor:1 | 1 (-1.14546) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12983 HOMO: -7.06952 LUMO: -2.08439 factor:1 | 1 (-1.38375) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25345 HOMO: -6.60965 LUMO: -2.11977 factor:1 | 1 (-1.50737) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13132 HOMO: -6.87360 LUMO: -1.85854 factor:1 | 1 (-1.38525) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10240 HOMO: -7.67089 LUMO: -0.24762 factor:1 | 1 (-1.35632) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02400 HOMO: -6.45726 LUMO: -1.86398 factor:1 | 1 (-1.27793) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03390 HOMO: -6.91713 LUMO: 0.33198 factor:1 | 1 (-2.28782) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15771 HOMO: -6.83278 LUMO: 0.26667 factor:1 | 1 (-2.41164) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13774 HOMO: -6.89264 LUMO: -1.00682 factor:1 | 1 (-2.39166) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.22013 HOMO: -6.57427 LUMO: 0.22041 factor:1 | 1 (-2.47406) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54939 HOMO: -7.52123 LUMO: -0.01905 factor:1 | 1 (-2.80332) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.39447 HOMO: -7.37429 LUMO: -0.08980 factor:1 | 1 (-2.64840) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.33744 HOMO: -7.28449 LUMO: -0.26395 factor:1 | 1 (-2.59137) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.57134 HOMO: -6.79740 LUMO: -0.60954 factor:1 | 1 (-3.82527) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56642 HOMO: -7.12666 LUMO: -0.60681 factor:1 | 1 (-2.82035) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54052 HOMO: -6.96611 LUMO: -0.30477 factor:1 | 1 (-2.79445) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57742 HOMO: -7.08040 LUMO: -0.31293 factor:1 | 1 (-2.83134) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.61663 HOMO: -6.78924 LUMO: -0.73743 factor:1 | 1 (-2.87056) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56936 HOMO: -7.57293 LUMO: -1.11295 factor:1 | 1 (-2.82329) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48024 HOMO: -7.15932 LUMO: -0.23130 factor:1 | 1 (-2.73417) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.39115 HOMO: -7.48585 LUMO: -0.10068 factor:1 | 1 (-2.64508) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31914 HOMO: -7.17020 LUMO: -0.26123 factor:1 | 1 (-0.57307) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21079 HOMO: -7.43143 LUMO: -0.16055 factor:1 | 1 (-0.46472) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38940 HOMO: -7.14843 LUMO: -0.10612 factor:1 | 1 (-0.64333) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73842 HOMO: -6.95523 LUMO: -0.22585 factor:1 | 1 (-0.99234) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65227 HOMO: -7.06680 LUMO: -0.51974 factor:1 | 1 (-0.90619) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75063 HOMO: -6.80829 LUMO: -0.64763 factor:1 | 1 (-1.00456) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62715 HOMO: -7.13210 LUMO: -0.48164 factor:1 | 1 (-0.88108) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79866 HOMO: -7.16204 LUMO: -0.45715 factor:1 | 1 (-1.05259) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90481 HOMO: -7.15115 LUMO: -0.43266 factor:1 | 1 (-1.15874) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22365 HOMO: -7.15932 LUMO: -2.52794 factor:1 | 1 (-1.47758) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08702 HOMO: -7.21102 LUMO: -2.65311 factor:1 | 1 (-1.34095) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04163 HOMO: -6.57427 LUMO: -2.78645 factor:1 | 1 (-1.29556) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02098 HOMO: -6.40828 LUMO: -3.23815 factor:1 | 1 (-1.27491) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.06265 HOMO: -7.71987 LUMO: -0.20953 factor:1 | 1 (-3.31658) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.76947 HOMO: -7.47769 LUMO: -0.43810 factor:1 | 1 (-4.02339) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64210 HOMO: -6.68040 LUMO: -2.22589 factor:1 | 1 (-2.89603) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12465 HOMO: -6.92802 LUMO: -1.99187 factor:1 | 1 (-2.37857) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.61561 HOMO: -7.73620 LUMO: 0.01633 factor:1 | 1 (-3.86954) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.59225 HOMO: -7.28721 LUMO: -0.18504 factor:1 | 1 (-2.84617) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60948 HOMO: -7.49674 LUMO: -0.19864 factor:1 | 1 (-1.86341) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.77734 HOMO: -7.10489 LUMO: -2.56331 factor:1 | 1 (-3.03127) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.76289 HOMO: -7.36612 LUMO: 0.16055 factor:1 | 1 (-3.01682) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30833 HOMO: -7.67633 LUMO: 0.33198 factor:1 | 1 (-1.56226) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.29072 HOMO: -7.07768 LUMO: -0.27483 factor:1 | 1 (-2.54465) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03681 HOMO: -7.32531 LUMO: 0.05442 factor:1 | 1 (-2.29074) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.46497 HOMO: -6.79740 LUMO: -1.21635 factor:1 | 1 (-3.71890) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.35681 HOMO: -7.14027 LUMO: 0.12517 factor:1 | 1 (-3.61073) | 1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11514.05472 HOMO: -7.17292 LUMO: 0.16871 factor:1 | 1 (-4.30865) | 1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.76275 HOMO: -7.08312 LUMO: -1.38778 factor:1 | 1 (-3.01668) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.75269 HOMO: -6.75387 LUMO: -1.88031 factor:1 | 1 (-3.00661) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.38472 HOMO: -7.07768 LUMO: -1.25717 factor:1 | 1 (-3.63865) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.18178 HOMO: -6.46543 LUMO: -1.14016 factor:1 | 1 (-3.43571) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89876 HOMO: -7.37973 LUMO: -0.45987 factor:1 | 1 (-2.15269) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11514.08455 HOMO: -7.46408 LUMO: 0.03265 factor:1 | 1 (-4.33847) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.38170 HOMO: -7.96477 LUMO: -0.19864 factor:1 | 1 (-3.63563) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.74403 HOMO: -6.93890 LUMO: -1.11839 factor:1 | 1 (-2.99796) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.84871 HOMO: -7.06408 LUMO: -1.08846 factor:1 | 1 (-3.10264) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57498 HOMO: -7.14027 LUMO: -0.33470 factor:1 | 1 (-1.82890) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.34279 HOMO: -7.38245 LUMO: 0.10885 factor:1 | 1 (-3.59672) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.61241 HOMO: -7.59470 LUMO: -1.21363 factor:1 | 1 (-2.86634) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55655 HOMO: -7.23279 LUMO: -1.23812 factor:1 | 1 (-2.81047) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62569 HOMO: -6.90897 LUMO: 0.23402 factor:1 | 1 (-2.87962) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21298 HOMO: -7.36340 LUMO: -0.17143 factor:1 | 1 (-1.46691) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89596 HOMO: -6.61781 LUMO: -0.01361 factor:1 | 1 (-2.14989) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60211 HOMO: -6.80013 LUMO: 0.38368 factor:1 | 1 (-1.85603) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.16421 HOMO: -6.72121 LUMO: -0.95512 factor:1 | 1 (-2.41814) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.22555 HOMO: -6.24773 LUMO: -0.69933 factor:1 | 1 (-2.47947) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.02829 HOMO: -6.56883 LUMO: 0.14694 factor:1 | 1 (-2.28222) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00562 HOMO: -6.51441 LUMO: -1.27621 factor:1 | 1 (-2.25955) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68894 HOMO: -6.91986 LUMO: -1.16737 factor:1 | 1 (-1.94287) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70344 HOMO: -6.17971 LUMO: -0.65307 factor:1 | 1 (-1.95737) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.93028 HOMO: -7.22462 LUMO: 0.04354 factor:1 | 1 (-1.18421) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.11501 HOMO: -7.16204 LUMO: -0.23674 factor:1 | 1 (-2.36894) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.29668 HOMO: -6.81645 LUMO: -0.19320 factor:1 | 1 (-2.55060) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.05001 HOMO: -6.69400 LUMO: 0.04082 factor:1 | 1 (-2.30393) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.28408 HOMO: -6.63141 LUMO: -0.22858 factor:1 | 1 (-2.53801) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81289 HOMO: -6.92258 LUMO: -1.11295 factor:1 | 1 (-2.06681) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28703 HOMO: -6.60148 LUMO: -1.13744 factor:1 | 1 (-1.54095) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55323 HOMO: -6.78108 LUMO: -0.82450 factor:1 | 1 (-2.80715) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48582 HOMO: -7.05591 LUMO: -0.97145 factor:1 | 1 (-2.73975) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03118 HOMO: -6.65318 LUMO: -1.26261 factor:1 | 1 (-2.28510) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.22587 HOMO: -6.98244 LUMO: -0.98233 factor:1 | 1 (-2.47980) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13488 HOMO: -7.11850 LUMO: -0.99594 factor:1 | 1 (-2.38881) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.05128 HOMO: -6.64230 LUMO: -0.93879 factor:1 | 1 (-2.30521) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26381 HOMO: -6.62053 LUMO: -1.22451 factor:1 | 1 (-2.51773) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26125 HOMO: -7.02598 LUMO: -0.85172 factor:1 | 1 (-2.51518) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93153 HOMO: -7.06680 LUMO: -0.89253 factor:1 | 1 (-2.18546) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61906 HOMO: -7.17292 LUMO: 0.00272 factor:1 | 1 (-1.87299) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62245 HOMO: -7.03142 LUMO: -0.35103 factor:1 | 1 (-2.87638) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.17141 HOMO: -6.96884 LUMO: -0.09796 factor:1 | 1 (-3.42534) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.44019 HOMO: -6.56339 LUMO: -0.99322 factor:1 | 1 (-2.69412) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.13443 HOMO: -7.08857 LUMO: -0.17687 factor:1 | 1 (-3.38836) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.42949 HOMO: -7.05863 LUMO: -0.22041 factor:1 | 1 (-3.68341) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.82934 HOMO: -7.15115 LUMO: -0.17960 factor:1 | 1 (-3.08327) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60055 HOMO: -6.67495 LUMO: -0.96600 factor:1 | 1 (-2.85447) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.32834 HOMO: -6.74026 LUMO: -1.79867 factor:1 | 1 (-3.58227) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91153 HOMO: -6.73482 LUMO: -1.78235 factor:1 | 1 (-2.16545) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90271 HOMO: -6.09807 LUMO: 0.16871 factor:1 | 1 (-2.15664) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97566 HOMO: -6.72393 LUMO: 0.27211 factor:1 | 1 (-2.22959) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48999 HOMO: -6.40556 LUMO: -0.04354 factor:1 | 1 (-2.74391) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54558 HOMO: -6.56883 LUMO: 0.22041 factor:1 | 1 (-2.79951) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.61812 HOMO: -7.22462 LUMO: 0.15783 factor:1 | 1 (-2.87205) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.12352 HOMO: -6.83550 LUMO: 0.19320 factor:1 | 1 (-3.37745) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.14031 HOMO: -7.26816 LUMO: -0.07619 factor:1 | 1 (-3.39424) | 1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60512 HOMO: -7.13483 LUMO: 0.33198 factor:1 | 1 (-2.85905) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.95155 HOMO: -6.58243 LUMO: -0.26395 factor:1 | 1 (-3.20547) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72335 HOMO: -7.38517 LUMO: 0.17143 factor:1 | 1 (-2.97728) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67881 HOMO: -6.80013 LUMO: 0.25851 factor:1 | 1 (-1.93274) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56148 HOMO: -6.96611 LUMO: 0.11429 factor:1 | 1 (-1.81541) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.33275 HOMO: -6.51713 LUMO: -1.14560 factor:1 | 1 (-3.58668) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.59363 HOMO: -7.15387 LUMO: -0.35647 factor:1 | 1 (-2.84756) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59345 HOMO: -5.26540 LUMO: 1.26805 factor:1 | 1 (-1.84738) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63185 HOMO: -6.76475 LUMO: -0.16327 factor:1 | 1 (-1.88578) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.14154 HOMO: -6.55250 LUMO: -0.71838 factor:1 | 1 (-3.39546) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.44060 HOMO: -6.76203 LUMO: -1.08301 factor:1 | 1 (-2.69453) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65903 HOMO: -7.14027 LUMO: -0.01633 factor:1 | 1 (-1.91296) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.41954 HOMO: -6.94979 LUMO: -0.93879 factor:1 | 1 (-2.67346) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55290 HOMO: -6.74842 LUMO: 0.31293 factor:1 | 1 (-2.80683) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41718 HOMO: -6.43821 LUMO: 0.05987 factor:1 | 1 (-1.67111) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.33212 HOMO: -6.60420 LUMO: 0.22585 factor:1 | 1 (-3.58605) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.69502 HOMO: -6.43821 LUMO: 0.05987 factor:1 | 1 (-2.94895) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.71102 HOMO: -6.34570 LUMO: 1.43948 factor:1 | 1 (-2.96495) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83191 HOMO: -6.03004 LUMO: 1.21363 factor:1 | 1 (-2.08583) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79495 HOMO: -6.68040 LUMO: -0.92247 factor:1 | 1 (-2.04888) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.06179 HOMO: -6.92530 LUMO: -0.31293 factor:1 | 1 (-2.31572) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97825 HOMO: -6.94979 LUMO: -0.19864 factor:1 | 1 (-2.23218) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.04968 HOMO: -6.80829 LUMO: -0.30477 factor:1 | 1 (-2.30361) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94747 HOMO: -7.22734 LUMO: -1.02859 factor:1 | 1 (-2.20140) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31189 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-2.56582) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.18108 HOMO: -7.27088 LUMO: -0.78097 factor:1 | 1 (-2.43501) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.37774 HOMO: -7.29809 LUMO: -0.97145 factor:1 | 1 (-2.63167) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84037 HOMO: -7.18925 LUMO: -0.94696 factor:1 | 1 (-2.09430) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90029 HOMO: -7.33891 LUMO: -0.96873 factor:1 | 1 (-2.15422) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90524 HOMO: -7.36068 LUMO: -0.28028 factor:1 | 1 (-2.15917) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60641 HOMO: -7.10761 LUMO: -1.14832 factor:1 | 1 (-1.86033) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.09813 HOMO: -6.94707 LUMO: -0.65307 factor:1 | 1 (-3.35206) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.11120 HOMO: -6.91713 LUMO: -1.81228 factor:1 | 1 (-3.36512) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.20924 HOMO: -6.78652 LUMO: -2.01636 factor:1 | 1 (-3.46317) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.80254 HOMO: -6.52801 LUMO: -1.17553 factor:1 | 1 (-3.05646) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90859 HOMO: -7.54844 LUMO: -1.18642 factor:1 | 1 (-2.16252) | 1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67501 HOMO: -7.52939 LUMO: -1.23812 factor:1 | 1 (-1.92893) | 1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.80390 HOMO: -7.94572 LUMO: -0.81634 factor:1 | 1 (-3.05783) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82080 HOMO: -7.55932 LUMO: -0.86260 factor:1 | 1 (-2.07473) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65002 HOMO: -7.72259 LUMO: -1.39050 factor:1 | 1 (-2.90394) | 1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62466 HOMO: -7.11850 LUMO: -1.01498 factor:1 | 1 (-2.87858) | 1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.82975 HOMO: -7.09673 LUMO: -1.00954 factor:1 | 1 (-3.08368) | 1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.15637 HOMO: -6.06270 LUMO: 0.16327 factor:1 | 1 (-3.41029) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50493 HOMO: -5.71167 LUMO: 0.70477 factor:1 | 1 (-2.75885) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30111 HOMO: -5.38241 LUMO: 0.86260 factor:1 | 1 (-2.55504) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.04809 HOMO: -5.67357 LUMO: 1.27621 factor:1 | 1 (-3.30202) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54574 HOMO: -7.56204 LUMO: -0.68573 factor:1 | 1 (-2.79967) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.12200 HOMO: -5.57833 LUMO: 1.13199 factor:1 | 1 (-3.37593) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.49196 HOMO: -7.58653 LUMO: -0.66124 factor:1 | 1 (-3.74589) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.78310 HOMO: -7.91851 LUMO: -1.10206 factor:1 | 1 (-4.03703) | 1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64046 HOMO: -6.48992 LUMO: -1.00138 factor:1 | 1 (-0.89438) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56873 HOMO: -7.09673 LUMO: -0.45171 factor:1 | 1 (-0.82265) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77621 HOMO: -6.63686 LUMO: 0.09252 factor:1 | 1 (-1.03014) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82317 HOMO: -6.84366 LUMO: -0.14422 factor:1 | 1 (-2.07710) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00260 HOMO: -6.93074 LUMO: 0.04354 factor:1 | 1 (-2.25653) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94622 HOMO: -6.90353 LUMO: -0.19864 factor:1 | 1 (-2.20015) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68667 HOMO: -6.59876 LUMO: -0.10068 factor:1 | 1 (-2.94060) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.31944 HOMO: -6.74570 LUMO: -0.44627 factor:1 | 1 (-3.57337) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.25033 HOMO: -6.60148 LUMO: -0.61770 factor:1 | 1 (-3.50426) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.66854 HOMO: -6.55794 LUMO: -1.06941 factor:1 | 1 (-3.92247) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77899 HOMO: -7.12666 LUMO: -0.11973 factor:1 | 1 (-1.03292) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76299 HOMO: -7.21646 LUMO: -0.50069 factor:1 | 1 (-1.01692) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43779 HOMO: -7.27632 LUMO: -1.00682 factor:1 | 1 (-0.69171) | 1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.61831 HOMO: -6.74298 LUMO: 0.04354 factor:1 | 1 (-0.87223) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57086 HOMO: -6.37291 LUMO: 0.14150 factor:1 | 1 (-2.82479) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.23472 HOMO: -5.61371 LUMO: 1.28438 factor:1 | -1 (0.51136) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.51556 HOMO: -5.52119 LUMO: 0.99866 factor:1 | -1 (0.23051) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.58604 HOMO: -6.51985 LUMO: -0.10885 factor:1 | 1 (-2.83997) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79082 HOMO: -5.61371 LUMO: 0.77280 factor:1 | 1 (-2.04475) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.27376 HOMO: -5.58922 LUMO: 0.24490 factor:1 | 1 (-0.52768) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.14973 HOMO: -6.32665 LUMO: -0.57144 factor:1 | 1 (-0.40365) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.26799 HOMO: -6.29127 LUMO: -0.93607 factor:1 | 1 (-0.52191) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57402 HOMO: -5.49670 LUMO: 0.27211 factor:1 | 1 (-1.82795) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.60193 HOMO: -5.68990 LUMO: 0.24218 factor:1 | 1 (-2.85586) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75707 HOMO: -5.68174 LUMO: 0.69933 factor:1 | 1 (-2.01100) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94015 HOMO: -5.28173 LUMO: 1.00954 factor:1 | 1 (-2.19408) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56257 HOMO: -5.94025 LUMO: 0.73471 factor:1 | 1 (-1.81650) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60485 HOMO: -5.65725 LUMO: 1.28710 factor:1 | 1 (-1.85878) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51072 HOMO: -5.41507 LUMO: 0.87076 factor:1 | 1 (-2.76465) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.12592 HOMO: -5.96474 LUMO: 0.29660 factor:1 | 1 (-0.37984) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38393 HOMO: -7.00421 LUMO: 0.08708 factor:1 | 1 (-0.63786) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75052 HOMO: -5.40418 LUMO: 0.90070 factor:1 | 1 (-2.00445) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88573 HOMO: -7.00421 LUMO: -0.30477 factor:1 | 1 (-2.13966) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.96946 HOMO: -5.85861 LUMO: 0.74015 factor:1 | 1 (-2.22339) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.50121 HOMO: -5.71439 LUMO: 0.26395 factor:1 | -1 (1.24487) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11507.81012 HOMO: -7.13755 LUMO: -0.78369 factor:1 | -1 (1.93595) | 1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.52861 HOMO: -7.31442 LUMO: -0.98233 factor:1 | -1 (1.21746) | 1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15328 HOMO: -7.25728 LUMO: -1.00410 factor:1 | 1 (-1.40721) | 1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17010 HOMO: -7.48585 LUMO: -0.83811 factor:1 | 1 (-1.42403) | 1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40621 HOMO: -7.24911 LUMO: -0.77280 factor:1 | 1 (-1.66014) | 1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56743 HOMO: -7.55116 LUMO: -1.19730 factor:1 | 1 (-2.82136) | 1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76603 HOMO: -5.76881 LUMO: 0.28028 factor:1 | 1 (-2.01996) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79585 HOMO: -5.77153 LUMO: -0.26939 factor:1 | 1 (-2.04978) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.22287 HOMO: -5.82868 LUMO: 0.36735 factor:1 | 1 (-0.47680) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10964 HOMO: -5.83140 LUMO: -0.17960 factor:1 | 1 (-0.36357) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88766 HOMO: -6.28855 LUMO: 0.01088 factor:1 | 1 (-2.14159) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78132 HOMO: -6.31576 LUMO: 0.25307 factor:1 | 1 (-2.03525) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.05689 HOMO: -7.06408 LUMO: -2.76196 factor:1 | 1 (-2.31082) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.69521 HOMO: -5.95657 LUMO: 0.37552 factor:1 | 1 (-2.94914) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49567 HOMO: -6.61781 LUMO: 0.02721 factor:1 | 1 (-2.74960) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42376 HOMO: -6.26678 LUMO: -0.66668 factor:1 | 1 (-1.67769) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26713 HOMO: -6.00011 LUMO: -0.13334 factor:1 | 1 (-1.52106) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46872 HOMO: -5.60555 LUMO: 0.67484 factor:1 | 1 (-1.72264) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72498 HOMO: -5.79875 LUMO: 0.99049 factor:1 | 1 (-2.97891) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28882 HOMO: -5.97834 LUMO: 0.48436 factor:1 | 1 (-1.54275) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32305 HOMO: -5.82868 LUMO: 0.91974 factor:1 | 1 (-1.57698) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60306 HOMO: -5.86677 LUMO: 0.99594 factor:1 | 1 (-1.85699) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38330 HOMO: -5.70079 LUMO: 0.48980 factor:1 | 1 (-1.63723) | -1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51680 HOMO: -7.39605 LUMO: -1.02315 factor:1 | 1 (-1.77073) | 1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55447 HOMO: -7.22734 LUMO: -1.12927 factor:1 | 1 (-0.80840) | 1 | -1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.82778 HOMO: -7.58926 LUMO: -0.65035 factor:1 | 1 (-1.08171) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.88598 HOMO: -7.43959 LUMO: -0.75648 factor:1 | 1 (-1.13991) | 1 | 1 |
| G: -5245.38038 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54039 HOMO: -7.55388 LUMO: -1.15104 factor:1 | 1 (-1.79432) | 1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42877 HOMO: -6.74570 LUMO: -2.85447 factor:1 | 1 (-1.68270) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52700 HOMO: -7.35524 LUMO: -1.25444 factor:1 | 1 (-1.78093) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.13628 HOMO: -6.81645 LUMO: -1.20819 factor:1 | 1 (-3.39021) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76301 HOMO: -6.99605 LUMO: -1.62996 factor:1 | 1 (-2.01694) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64953 HOMO: -6.88992 LUMO: -0.47620 factor:1 | 1 (-2.90345) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72184 HOMO: -7.22190 LUMO: -0.01905 factor:1 | 1 (-1.97576) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.33472 HOMO: -6.77836 LUMO: -0.82995 factor:1 | 1 (-2.58865) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.24062 HOMO: -6.48447 LUMO: -0.95512 factor:1 | 1 (-2.49455) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.63611 HOMO: -7.81239 LUMO: 1.22179 factor:1 | 1 (-2.89004) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.78651 HOMO: -7.36612 LUMO: 0.19320 factor:1 | 1 (-3.04044) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.46162 HOMO: -7.24095 LUMO: 0.33470 factor:1 | 1 (-3.71555) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76887 HOMO: -7.15932 LUMO: -2.24222 factor:1 | 1 (-1.02279) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64742 HOMO: -6.88992 LUMO: -2.69937 factor:1 | 1 (-0.90135) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62078 HOMO: -6.97428 LUMO: -0.98233 factor:1 | 1 (-0.87471) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49659 HOMO: -7.17564 LUMO: -0.93879 factor:1 | 1 (-0.75052) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34265 HOMO: -6.81645 LUMO: -1.14288 factor:1 | 1 (-0.59658) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.70931 HOMO: -6.83006 LUMO: -0.63403 factor:1 | -1 (0.03676) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.02096 HOMO: -7.17292 LUMO: -1.07213 factor:1 | 1 (-0.27489) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.65339 HOMO: -7.53755 LUMO: 0.15510 factor:1 | -1 (0.09268) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.96964 HOMO: -6.50080 LUMO: -0.51702 factor:1 | 1 (-0.22357) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43270 HOMO: -6.72665 LUMO: -0.80001 factor:1 | 1 (-0.68662) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59890 HOMO: -6.72665 LUMO: 1.68711 factor:1 | 1 (-0.85283) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.69551 HOMO: -7.11850 LUMO: -0.75103 factor:1 | -1 (0.05056) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.48378 HOMO: -6.87087 LUMO: -0.85988 factor:1 | -1 (0.26229) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99338 HOMO: -7.08857 LUMO: -0.89798 factor:1 | 1 (-2.24731) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93485 HOMO: -6.71305 LUMO: -0.85444 factor:1 | 1 (-2.18878) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.59630 HOMO: -6.59332 LUMO: -0.60137 factor:1 | 1 (-2.85023) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.96791 HOMO: -7.28993 LUMO: 0.03265 factor:1 | 1 (-2.22184) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39339 HOMO: -7.32258 LUMO: 0.13878 factor:1 | 1 (-1.64732) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41470 HOMO: -7.28993 LUMO: 0.11429 factor:1 | 1 (-1.66863) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20672 HOMO: -6.86271 LUMO: -1.03947 factor:1 | 1 (-1.46065) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17949 HOMO: -6.55794 LUMO: -0.84900 factor:1 | 1 (-1.43341) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06308 HOMO: -7.03686 LUMO: 0.11429 factor:1 | 1 (-1.31700) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.98680 HOMO: -7.06952 LUMO: -0.96056 factor:1 | 1 (-1.24073) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09872 HOMO: -6.90897 LUMO: -0.99866 factor:1 | 1 (-1.35265) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72889 HOMO: -7.00693 LUMO: -0.83539 factor:1 | 1 (-0.98282) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03603 HOMO: -6.74298 LUMO: -0.85172 factor:1 | 1 (-1.28996) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67790 HOMO: -6.83822 LUMO: -1.07213 factor:1 | 1 (-0.93183) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67335 HOMO: -7.21918 LUMO: -1.55377 factor:1 | 1 (-0.92728) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55433 HOMO: -6.84094 LUMO: -1.09934 factor:1 | 1 (-0.80826) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49662 HOMO: -7.09129 LUMO: -0.85988 factor:1 | 1 (-0.75054) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52753 HOMO: -6.57971 LUMO: -2.27215 factor:1 | 1 (-0.78146) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76219 HOMO: -6.81373 LUMO: -1.86942 factor:1 | 1 (-2.01612) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72018 HOMO: -6.59060 LUMO: -2.30480 factor:1 | 1 (-1.97410) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73375 HOMO: -6.72938 LUMO: -1.23540 factor:1 | 1 (-1.98768) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64007 HOMO: -6.94707 LUMO: -2.62318 factor:1 | 1 (-1.89399) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36613 HOMO: -7.28177 LUMO: -0.09796 factor:1 | 1 (-1.62006) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55487 HOMO: -6.80013 LUMO: -0.79729 factor:1 | 1 (-1.80880) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73430 HOMO: -7.26544 LUMO: 0.12789 factor:1 | 1 (-1.98823) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56952 HOMO: -6.51713 LUMO: -0.49253 factor:1 | 1 (-0.82344) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55939 HOMO: -6.68856 LUMO: -0.77280 factor:1 | 1 (-0.81332) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54590 HOMO: -6.41100 LUMO: -0.70750 factor:1 | 1 (-0.79982) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44802 HOMO: -7.56204 LUMO: 0.22041 factor:1 | 1 (-0.70194) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.28548 HOMO: -6.68312 LUMO: 1.30343 factor:1 | 1 (-0.53941) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.45275 HOMO: -7.24367 LUMO: 0.17415 factor:1 | 1 (-0.70668) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.74598 HOMO: -7.52395 LUMO: 1.16737 factor:1 | 1 (-0.99991) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63099 HOMO: -6.89264 LUMO: 0.23130 factor:1 | 1 (-0.88491) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.61025 HOMO: -7.21102 LUMO: 0.19048 factor:1 | 1 (-0.86418) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92429 HOMO: -7.08312 LUMO: 0.25034 factor:1 | 1 (-2.17822) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78687 HOMO: -6.49536 LUMO: -0.65852 factor:1 | 1 (-2.04080) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88453 HOMO: -6.85455 LUMO: 0.13606 factor:1 | 1 (-2.13846) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85211 HOMO: -7.10217 LUMO: 0.35919 factor:1 | 1 (-1.10603) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18566 HOMO: -7.77429 LUMO: 1.19186 factor:1 | 1 (-1.43959) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.67630 HOMO: -6.57427 LUMO: -0.50069 factor:1 | 1 (-2.93023) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.58664 HOMO: -7.36340 LUMO: 0.10068 factor:1 | 1 (-2.84057) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45358 HOMO: -7.28177 LUMO: 0.15238 factor:1 | 1 (-2.70751) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.23604 HOMO: -6.86543 LUMO: -0.84355 factor:1 | 1 (-3.48997) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84810 HOMO: -6.55794 LUMO: 1.39594 factor:1 | 1 (-2.10203) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71596 HOMO: -6.26134 LUMO: 1.53744 factor:1 | 1 (-1.96989) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88799 HOMO: -5.97562 LUMO: 1.42316 factor:1 | 1 (-2.14192) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92418 HOMO: -6.65046 LUMO: 1.44492 factor:1 | 1 (-2.17811) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99766 HOMO: -6.92258 LUMO: 0.17415 factor:1 | 1 (-1.25159) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09268 HOMO: -7.40966 LUMO: 0.19592 factor:1 | 1 (-1.34661) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.64362 HOMO: -7.17564 LUMO: 0.16871 factor:1 | -1 (0.10245) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.86384 HOMO: -7.46953 LUMO: 0.22313 factor:1 | 1 (-0.11777) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53417 HOMO: -6.13345 LUMO: 1.85854 factor:1 | 1 (-0.78810) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68238 HOMO: -6.99333 LUMO: -1.65717 factor:1 | 1 (-1.93631) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53470 HOMO: -6.93074 LUMO: -1.79323 factor:1 | 1 (-1.78863) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62502 HOMO: -6.87904 LUMO: -1.79323 factor:1 | 1 (-1.87895) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33211 HOMO: -6.84094 LUMO: 0.66940 factor:1 | 1 (-1.58604) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62426 HOMO: -7.13210 LUMO: -1.17553 factor:1 | 1 (-1.87818) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59049 HOMO: -6.52801 LUMO: -2.23678 factor:1 | 1 (-1.84441) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74067 HOMO: -6.81917 LUMO: -1.86398 factor:1 | 1 (-1.99459) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84331 HOMO: -7.30626 LUMO: -1.66806 factor:1 | 1 (-2.09724) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34172 HOMO: -6.98516 LUMO: -1.40683 factor:1 | 1 (-1.59565) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55884 HOMO: -6.95523 LUMO: -0.97145 factor:1 | 1 (-1.81277) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40806 HOMO: -6.83278 LUMO: -2.68848 factor:1 | 1 (-1.66199) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34490 HOMO: -7.25456 LUMO: -2.97420 factor:1 | 1 (-1.59883) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49567 HOMO: -6.80557 LUMO: -2.65039 factor:1 | 1 (-2.74960) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.27601 HOMO: -7.10489 LUMO: 0.77008 factor:1 | 1 (-3.52994) | 1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56117 HOMO: -7.28993 LUMO: -1.06124 factor:1 | 1 (-2.81510) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79337 HOMO: -7.11578 LUMO: -1.10206 factor:1 | 1 (-2.04730) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75166 HOMO: -6.91713 LUMO: -1.36329 factor:1 | 1 (-2.00559) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80785 HOMO: -7.07224 LUMO: 0.51974 factor:1 | 1 (-2.06178) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39288 HOMO: -7.22734 LUMO: -0.93335 factor:1 | 1 (-1.64681) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35612 HOMO: -7.19469 LUMO: -0.96600 factor:1 | 1 (-1.61004) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.68847 HOMO: -6.93890 LUMO: -0.66940 factor:1 | -1 (0.05761) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.67187 HOMO: -7.09673 LUMO: -1.05852 factor:1 | -1 (0.07421) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.31722 HOMO: -7.19197 LUMO: -2.26943 factor:1 | -1 (0.42885) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63627 HOMO: -6.90081 LUMO: -2.64767 factor:1 | 1 (-0.89019) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64671 HOMO: -6.93890 LUMO: -2.65039 factor:1 | 1 (-0.90064) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.75726 HOMO: -6.80013 LUMO: -2.54154 factor:1 | 1 (-0.01118) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76636 HOMO: -6.68040 LUMO: -0.89798 factor:1 | 1 (-1.02029) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59368 HOMO: -7.01782 LUMO: -1.09662 factor:1 | 1 (-0.84761) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.18573 HOMO: -6.58516 LUMO: -0.83539 factor:1 | 1 (-0.43965) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.07655 HOMO: -7.46953 LUMO: 0.06259 factor:1 | 1 (-0.33048) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.23269 HOMO: -6.96884 LUMO: -0.99866 factor:1 | 1 (-0.48662) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.12374 HOMO: -7.29809 LUMO: -0.19320 factor:1 | 1 (-0.37767) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40929 HOMO: -6.86271 LUMO: 0.04082 factor:1 | 1 (-0.66322) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59069 HOMO: -6.36746 LUMO: -1.02587 factor:1 | 1 (-0.84461) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37626 HOMO: -7.15659 LUMO: -1.25989 factor:1 | 1 (-0.63019) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.15819 HOMO: -6.69128 LUMO: -0.59865 factor:1 | 1 (-0.41212) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.99631 HOMO: -7.09129 LUMO: -1.08573 factor:1 | 1 (-0.25024) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.24130 HOMO: -6.64502 LUMO: -0.66396 factor:1 | -1 (0.50477) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44135 HOMO: -6.93346 LUMO: -0.87349 factor:1 | 1 (-0.69528) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19136 HOMO: -6.77019 LUMO: -0.87349 factor:1 | 1 (-0.44529) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29373 HOMO: -6.59060 LUMO: -0.82995 factor:1 | 1 (-0.54766) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50983 HOMO: -7.17564 LUMO: -1.08846 factor:1 | 1 (-1.76376) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30485 HOMO: -7.27088 LUMO: -1.18642 factor:1 | 1 (-1.55878) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37764 HOMO: -7.06680 LUMO: -1.13199 factor:1 | 1 (-1.63157) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12493 HOMO: -7.21918 LUMO: -1.03947 factor:1 | 1 (-1.37886) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85842 HOMO: -7.26000 LUMO: -0.11973 factor:1 | 1 (-1.11235) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84242 HOMO: -6.77564 LUMO: 0.23402 factor:1 | 1 (-1.09635) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52266 HOMO: -7.07224 LUMO: -0.75648 factor:1 | 1 (-0.77659) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52660 HOMO: -7.45048 LUMO: 0.18232 factor:1 | 1 (-0.78053) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63746 HOMO: -7.48313 LUMO: 0.15238 factor:1 | 1 (-0.89139) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31710 HOMO: -6.60692 LUMO: -0.50885 factor:1 | 1 (-0.57103) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31533 HOMO: -6.62869 LUMO: -0.60954 factor:1 | 1 (-0.56926) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.03998 HOMO: -7.40422 LUMO: -1.28982 factor:1 | 1 (-0.29391) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.87807 HOMO: -6.75114 LUMO: -1.23268 factor:1 | 1 (-0.13200) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.97965 HOMO: -6.84638 LUMO: -0.73199 factor:1 | 1 (-0.23358) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.72765 HOMO: -6.79196 LUMO: -1.43676 factor:1 | -1 (0.01842) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.76441 HOMO: -7.00965 LUMO: -1.37690 factor:1 | 1 (-0.01834) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.08798 HOMO: -6.97972 LUMO: -1.58098 factor:1 | 1 (-0.34191) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.83119 HOMO: -6.91169 LUMO: -1.48574 factor:1 | 1 (-0.08512) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.53516 HOMO: -6.90081 LUMO: -1.30343 factor:1 | -1 (0.21092) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62010 HOMO: -6.78652 LUMO: -1.51840 factor:1 | 1 (-0.87403) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41066 HOMO: -6.84638 LUMO: -1.15104 factor:1 | 1 (-0.66458) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50562 HOMO: -6.61237 LUMO: -0.89798 factor:1 | 1 (-0.75955) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46516 HOMO: -7.16204 LUMO: -1.30070 factor:1 | 1 (-0.71909) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44834 HOMO: -7.32803 LUMO: 0.14694 factor:1 | 1 (-0.70227) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33835 HOMO: -6.99877 LUMO: -0.87621 factor:1 | 1 (-0.59228) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.89865 HOMO: -6.99877 LUMO: -0.97145 factor:1 | 1 (-0.15257) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.92561 HOMO: -7.08040 LUMO: -1.09662 factor:1 | 1 (-0.17954) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.00722 HOMO: -6.90897 LUMO: -1.14016 factor:1 | 1 (-0.26115) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.57158 HOMO: -6.68312 LUMO: -0.74831 factor:1 | 1 (-0.82551) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37871 HOMO: -6.99061 LUMO: -0.86804 factor:1 | 1 (-0.63264) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51077 HOMO: -7.10761 LUMO: -1.18642 factor:1 | 1 (-0.76469) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.86311 HOMO: -6.79196 LUMO: -0.71294 factor:1 | 1 (-0.11704) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11717 HOMO: -6.86271 LUMO: -0.81362 factor:1 | 1 (-1.37110) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14109 HOMO: -7.01510 LUMO: -0.99322 factor:1 | 1 (-1.39502) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04678 HOMO: -6.88720 LUMO: -0.87893 factor:1 | 1 (-1.30070) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21143 HOMO: -6.88448 LUMO: 0.22041 factor:1 | 1 (-1.46536) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64195 HOMO: -7.55932 LUMO: 1.12111 factor:1 | 1 (-0.89588) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59417 HOMO: -6.46815 LUMO: -0.86260 factor:1 | 1 (-0.84810) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.45185 HOMO: -7.13755 LUMO: 0.23130 factor:1 | 1 (-0.70578) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50625 HOMO: -6.78924 LUMO: 1.51023 factor:1 | 1 (-0.76018) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37700 HOMO: -6.48992 LUMO: 1.74969 factor:1 | 1 (-0.63092) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60867 HOMO: -6.78380 LUMO: 1.81500 factor:1 | 1 (-0.86260) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60745 HOMO: -6.49536 LUMO: 1.70615 factor:1 | 1 (-0.86138) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04762 HOMO: -6.38651 LUMO: 1.44492 factor:1 | 1 (-1.30155) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33440 HOMO: -6.83822 LUMO: 1.38234 factor:1 | 1 (-1.58833) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.80650 HOMO: -6.01644 LUMO: 1.20274 factor:1 | 1 (-1.06043) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.78898 HOMO: -6.18243 LUMO: 1.77962 factor:1 | 1 (-1.04290) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99328 HOMO: -6.81917 LUMO: -1.01771 factor:1 | 1 (-1.24721) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04201 HOMO: -6.61237 LUMO: -0.91702 factor:1 | 1 (-1.29594) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27761 HOMO: -6.84094 LUMO: -0.84900 factor:1 | 1 (-1.53154) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29493 HOMO: -6.81917 LUMO: -1.01771 factor:1 | 1 (-0.54885) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41803 HOMO: -7.86953 LUMO: 1.16737 factor:1 | 1 (-0.67196) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41550 HOMO: -7.40694 LUMO: 0.11429 factor:1 | 1 (-0.66943) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72922 HOMO: -6.70489 LUMO: -0.65035 factor:1 | 1 (-0.98315) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36099 HOMO: -7.23279 LUMO: 0.33470 factor:1 | 1 (-0.61492) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56369 HOMO: -7.17020 LUMO: 0.41361 factor:1 | 1 (-0.81762) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43607 HOMO: -6.90353 LUMO: -0.90070 factor:1 | 1 (-0.69000) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33104 HOMO: -7.39061 LUMO: 0.17687 factor:1 | 1 (-0.58496) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12968 HOMO: -7.16748 LUMO: 0.42178 factor:1 | 1 (-2.38361) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.04562 HOMO: -7.36884 LUMO: -1.11295 factor:1 | 1 (-2.29955) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15583 HOMO: -7.33347 LUMO: 0.33198 factor:1 | 1 (-2.40976) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82943 HOMO: -7.31986 LUMO: -0.83539 factor:1 | 1 (-2.08336) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03014 HOMO: -7.31170 LUMO: 0.08708 factor:1 | 1 (-2.28407) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91308 HOMO: -7.36884 LUMO: 0.38096 factor:1 | 1 (-2.16701) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14016 HOMO: -6.99333 LUMO: 1.74153 factor:1 | 1 (-2.39408) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83610 HOMO: -6.94435 LUMO: 1.74969 factor:1 | 1 (-2.09002) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00181 HOMO: -7.02598 LUMO: 1.43404 factor:1 | 1 (-2.25574) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.04271 HOMO: -6.41100 LUMO: 1.62996 factor:1 | 1 (-2.29664) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97327 HOMO: -6.57699 LUMO: 1.81228 factor:1 | 1 (-2.22720) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67345 HOMO: -6.86543 LUMO: 1.49935 factor:1 | 1 (-1.92738) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89735 HOMO: -6.91169 LUMO: -1.22451 factor:1 | 1 (-2.15128) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00832 HOMO: -7.09945 LUMO: -1.23812 factor:1 | 1 (-2.26225) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92056 HOMO: -7.48857 LUMO: 0.10340 factor:1 | 1 (-2.17449) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.06330 HOMO: -7.21918 LUMO: -0.06803 factor:1 | 1 (-0.31723) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.03546 HOMO: -6.34025 LUMO: -0.68845 factor:1 | 1 (-0.28939) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.81350 HOMO: -6.82734 LUMO: -0.77825 factor:1 | 1 (-0.06743) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.08978 HOMO: -6.92258 LUMO: -1.03675 factor:1 | 1 (-0.34371) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.76670 HOMO: -6.42461 LUMO: -0.95240 factor:1 | 1 (-0.02063) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.80274 HOMO: -6.96067 LUMO: -1.05036 factor:1 | 1 (-1.05667) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66054 HOMO: -7.23551 LUMO: 0.12245 factor:1 | 1 (-0.91447) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.68018 HOMO: -6.85183 LUMO: 0.16055 factor:1 | 1 (-0.93411) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83246 HOMO: -6.46815 LUMO: -0.89253 factor:1 | 1 (-1.08639) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08389 HOMO: -7.23823 LUMO: -0.06259 factor:1 | 1 (-1.33782) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76655 HOMO: -6.76475 LUMO: -0.99049 factor:1 | 1 (-1.02048) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03184 HOMO: -7.14843 LUMO: -0.88165 factor:1 | 1 (-1.28577) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.28336 HOMO: -7.15659 LUMO: 0.20681 factor:1 | 1 (-0.53729) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81469 HOMO: -7.11306 LUMO: 0.14150 factor:1 | 1 (-1.06862) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.01215 HOMO: -6.67223 LUMO: -0.86260 factor:1 | 1 (-2.26608) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.96138 HOMO: -6.92530 LUMO: 0.30749 factor:1 | 1 (-2.21531) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85550 HOMO: -6.50624 LUMO: -0.70477 factor:1 | 1 (-2.10943) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.73492 HOMO: -7.35524 LUMO: 0.75103 factor:1 | -1 (0.01116) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.75130 HOMO: -7.07768 LUMO: -0.26939 factor:1 | 1 (-0.00522) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.06474 HOMO: -7.15932 LUMO: 0.42450 factor:1 | 1 (-0.31867) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55409 HOMO: -7.46136 LUMO: 0.04626 factor:1 | 1 (-0.80801) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56935 HOMO: -7.05047 LUMO: -1.06669 factor:1 | 1 (-0.82328) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00797 HOMO: -6.66951 LUMO: -0.99322 factor:1 | 1 (-1.26190) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19483 HOMO: -7.01782 LUMO: -1.08846 factor:1 | 1 (-1.44876) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99099 HOMO: -7.03959 LUMO: -1.15376 factor:1 | 1 (-1.24492) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42067 HOMO: -6.68856 LUMO: 1.61364 factor:1 | 1 (-0.67460) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49009 HOMO: -6.53345 LUMO: 1.60275 factor:1 | 1 (-0.74401) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32420 HOMO: -6.73482 LUMO: 1.86398 factor:1 | 1 (-1.57812) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.91099 HOMO: -6.87632 LUMO: 1.59731 factor:1 | 1 (-1.16492) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.16974 HOMO: -6.31848 LUMO: 2.12521 factor:1 | 1 (-1.42367) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.98185 HOMO: -6.35114 LUMO: 1.71432 factor:1 | 1 (-1.23578) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14923 HOMO: -6.34842 LUMO: 1.92929 factor:1 | 1 (-1.40316) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43130 HOMO: -6.14977 LUMO: 1.78235 factor:1 | 1 (-1.68523) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.05967 HOMO: -6.31032 LUMO: 1.51567 factor:1 | 1 (-1.31360) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44058 HOMO: -6.25862 LUMO: 1.75241 factor:1 | 1 (-1.69451) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18066 HOMO: -6.49264 LUMO: 1.66806 factor:1 | 1 (-1.43458) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10672 HOMO: -6.28311 LUMO: 1.60003 factor:1 | 1 (-1.36065) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.05388 HOMO: -7.13210 LUMO: -0.04354 factor:1 | 1 (-1.30781) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99129 HOMO: -7.35252 LUMO: 0.03537 factor:1 | 1 (-1.24522) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29116 HOMO: -6.58243 LUMO: -0.48980 factor:1 | 1 (-1.54509) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.68584 HOMO: -6.90081 LUMO: -0.05442 factor:1 | 1 (-0.93977) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84027 HOMO: -7.22734 LUMO: 0.17143 factor:1 | 1 (-1.09420) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70329 HOMO: -7.13210 LUMO: -0.99866 factor:1 | 1 (-0.95721) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.92258 HOMO: -7.39878 LUMO: 0.13334 factor:1 | 1 (-1.17651) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83115 HOMO: -7.04503 LUMO: -0.89798 factor:1 | 1 (-1.08508) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84966 HOMO: -6.95523 LUMO: -1.07213 factor:1 | 1 (-1.10358) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06925 HOMO: -6.75114 LUMO: -1.28438 factor:1 | 1 (-1.32318) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.97770 HOMO: -6.75114 LUMO: -0.11701 factor:1 | 1 (-0.23162) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19288 HOMO: -6.83278 LUMO: -0.01633 factor:1 | 1 (-0.44681) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.95922 HOMO: -6.93890 LUMO: -0.88981 factor:1 | 1 (-0.21315) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.96504 HOMO: -7.07224 LUMO: -1.08573 factor:1 | 1 (-0.21897) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.08504 HOMO: -6.99877 LUMO: -0.95240 factor:1 | 1 (-0.33897) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.61096 HOMO: -7.09129 LUMO: 0.35375 factor:1 | 1 (-0.86489) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58081 HOMO: -7.09401 LUMO: 0.04354 factor:1 | 1 (-0.83474) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55651 HOMO: -6.85183 LUMO: -0.68573 factor:1 | 1 (-0.81044) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84200 HOMO: -6.83006 LUMO: -0.58777 factor:1 | 1 (-2.09593) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21277 HOMO: -7.40422 LUMO: 0.17687 factor:1 | 1 (-1.46669) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84995 HOMO: -7.15932 LUMO: 0.10340 factor:1 | 1 (-2.10388) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65895 HOMO: -7.03414 LUMO: -0.19592 factor:1 | 1 (-1.91288) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74020 HOMO: -6.48447 LUMO: -0.36191 factor:1 | 1 (-1.99413) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60785 HOMO: -7.49402 LUMO: 0.11429 factor:1 | 1 (-1.86178) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62962 HOMO: -7.01237 LUMO: -1.06397 factor:1 | 1 (-1.88354) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15206 HOMO: -6.67223 LUMO: -1.07213 factor:1 | 1 (-1.40599) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06833 HOMO: -7.38789 LUMO: -1.15376 factor:1 | 1 (-1.32226) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07472 HOMO: -6.42461 LUMO: -1.23812 factor:1 | 1 (-1.32865) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79898 HOMO: -7.36884 LUMO: -1.19186 factor:1 | 1 (-2.05291) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50703 HOMO: -6.65591 LUMO: 0.07075 factor:1 | 1 (-1.76096) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80527 HOMO: -7.39061 LUMO: -0.16871 factor:1 | 1 (-2.05919) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.53434 HOMO: -6.90353 LUMO: -0.96056 factor:1 | 1 (-2.78827) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50272 HOMO: -7.42054 LUMO: 0.19048 factor:1 | 1 (-2.75665) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.02121 HOMO: -7.40150 LUMO: 0.35647 factor:1 | 1 (-3.27514) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.16666 HOMO: -6.56067 LUMO: -0.96056 factor:1 | 1 (-2.42059) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.67162 HOMO: -6.89809 LUMO: -0.81090 factor:1 | 1 (-2.92555) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62702 HOMO: -6.91986 LUMO: -0.84900 factor:1 | 1 (-2.88095) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57002 HOMO: -6.61509 LUMO: -0.62042 factor:1 | 1 (-2.82394) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.26197 HOMO: -6.58243 LUMO: -0.65579 factor:1 | 1 (-3.51590) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.15612 HOMO: -6.52257 LUMO: -0.92519 factor:1 | 1 (-3.41005) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.33072 HOMO: -6.69128 LUMO: 1.49118 factor:1 | 1 (-2.58465) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.24449 HOMO: -7.02870 LUMO: 1.67894 factor:1 | 1 (-2.49841) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.47562 HOMO: -6.88720 LUMO: 1.68711 factor:1 | 1 (-2.72955) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34678 HOMO: -5.89943 LUMO: 1.03675 factor:1 | 1 (-1.60071) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29032 HOMO: -6.40556 LUMO: 1.14560 factor:1 | 1 (-1.54425) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13301 HOMO: -6.51168 LUMO: 1.48030 factor:1 | 1 (-1.38694) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86864 HOMO: -6.64502 LUMO: 1.91568 factor:1 | 1 (-2.12257) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51867 HOMO: -6.47903 LUMO: 1.91296 factor:1 | 1 (-2.77260) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.36163 HOMO: -6.34297 LUMO: 1.91840 factor:1 | 1 (-2.61556) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50250 HOMO: -6.89809 LUMO: 1.82861 factor:1 | 1 (-2.75643) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66132 HOMO: -6.10079 LUMO: 1.62996 factor:1 | 1 (-1.91525) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40167 HOMO: -7.16476 LUMO: -0.92247 factor:1 | 1 (-1.65560) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55332 HOMO: -7.10489 LUMO: -0.95784 factor:1 | 1 (-1.80724) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.04867 HOMO: -6.76475 LUMO: -0.99866 factor:1 | 1 (-2.30260) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74518 HOMO: -6.81373 LUMO: -1.05036 factor:1 | 1 (-1.99911) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.09616 HOMO: -6.90081 LUMO: -1.03947 factor:1 | 1 (-2.35008) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56254 HOMO: -7.06952 LUMO: -0.91702 factor:1 | 1 (-1.81647) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63762 HOMO: -6.73482 LUMO: -0.94151 factor:1 | 1 (-1.89155) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73895 HOMO: -6.99605 LUMO: -1.04764 factor:1 | 1 (-1.99288) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32839 HOMO: -7.03686 LUMO: -0.93335 factor:1 | 1 (-1.58231) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08965 HOMO: -6.81101 LUMO: -0.95240 factor:1 | 1 (-2.34358) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85027 HOMO: -6.83822 LUMO: -0.65307 factor:1 | 1 (-2.10420) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72911 HOMO: -7.05319 LUMO: -0.81634 factor:1 | 1 (-0.98304) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.95496 HOMO: -7.57565 LUMO: 0.19048 factor:1 | 1 (-1.20889) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76326 HOMO: -6.56067 LUMO: -0.50613 factor:1 | 1 (-1.01719) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69457 HOMO: -6.74298 LUMO: -0.70477 factor:1 | 1 (-1.94850) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89906 HOMO: -7.02054 LUMO: 0.03537 factor:1 | 1 (-2.15299) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69824 HOMO: -7.33347 LUMO: -0.17960 factor:1 | 1 (-1.95217) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.97010 HOMO: -6.98244 LUMO: -0.88165 factor:1 | 1 (-3.22403) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48833 HOMO: -7.14843 LUMO: -1.19730 factor:1 | 1 (-2.74225) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50201 HOMO: -7.17564 LUMO: -1.21907 factor:1 | 1 (-2.75594) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.99990 HOMO: -6.74026 LUMO: -0.86532 factor:1 | 1 (-0.25383) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34113 HOMO: -6.82462 LUMO: -1.24084 factor:1 | 1 (-0.59506) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.18148 HOMO: -6.78924 LUMO: -0.70477 factor:1 | 1 (-0.43541) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44240 HOMO: -7.41238 LUMO: 0.05987 factor:1 | 1 (-1.69633) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38319 HOMO: -6.75931 LUMO: 0.02721 factor:1 | 1 (-1.63712) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10667 HOMO: -6.28583 LUMO: -0.93063 factor:1 | 1 (-1.36060) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88412 HOMO: -6.69128 LUMO: -0.83539 factor:1 | 1 (-2.13805) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13036 HOMO: -7.22190 LUMO: 0.01361 factor:1 | 1 (-2.38429) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90328 HOMO: -6.95251 LUMO: -1.09934 factor:1 | 1 (-2.15721) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03826 HOMO: -6.75387 LUMO: -0.90614 factor:1 | 1 (-1.29219) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.13734 HOMO: -7.48585 LUMO: 0.05987 factor:1 | 1 (-1.39126) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45728 HOMO: -6.92802 LUMO: -0.66940 factor:1 | 1 (-2.71121) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.24087 HOMO: -7.29537 LUMO: -0.14150 factor:1 | 1 (-2.49479) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.78724 HOMO: -6.57155 LUMO: -0.86804 factor:1 | 1 (-3.04117) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.44999 HOMO: -6.87632 LUMO: -0.77825 factor:1 | 1 (-2.70391) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31448 HOMO: -6.45998 LUMO: -0.31565 factor:1 | 1 (-1.56841) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15932 HOMO: -7.51306 LUMO: 0.05714 factor:1 | 1 (-1.41325) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72712 HOMO: -6.86271 LUMO: -0.00816 factor:1 | 1 (-0.98105) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84217 HOMO: -6.43277 LUMO: -1.07485 factor:1 | 1 (-1.09610) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58968 HOMO: -6.78108 LUMO: -0.81362 factor:1 | 1 (-0.84361) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51980 HOMO: -6.88448 LUMO: 1.21907 factor:1 | 1 (-0.77373) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65085 HOMO: -6.97700 LUMO: 1.44765 factor:1 | 1 (-0.90478) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.89927 HOMO: -6.89537 LUMO: 2.12249 factor:1 | 1 (-0.15320) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.73973 HOMO: -6.28311 LUMO: 1.45037 factor:1 | -1 (0.00634) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.90061 HOMO: -6.55522 LUMO: 1.39867 factor:1 | 1 (-0.15453) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.59031 HOMO: -6.46815 LUMO: 1.50207 factor:1 | -1 (0.15576) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.98542 HOMO: -6.43549 LUMO: 2.17419 factor:1 | 1 (-0.23935) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85823 HOMO: -6.99333 LUMO: 1.87214 factor:1 | 1 (-1.11216) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.87145 HOMO: -6.65591 LUMO: 1.37962 factor:1 | 1 (-1.12538) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63455 HOMO: -6.82734 LUMO: 1.55649 factor:1 | 1 (-0.88848) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19124 HOMO: -6.71849 LUMO: 1.36057 factor:1 | 1 (-1.44517) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19448 HOMO: -6.79468 LUMO: 1.82044 factor:1 | 1 (-1.44841) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71892 HOMO: -6.61237 LUMO: 1.15104 factor:1 | 1 (-1.97285) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81248 HOMO: -6.62053 LUMO: 2.33474 factor:1 | 1 (-2.06641) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31012 HOMO: -6.55794 LUMO: 1.65717 factor:1 | 1 (-2.56405) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.86115 HOMO: -6.85999 LUMO: 2.03813 factor:1 | 1 (-3.11508) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31842 HOMO: -6.45726 LUMO: 1.28438 factor:1 | 1 (-2.57235) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20106 HOMO: -6.23685 LUMO: 1.93201 factor:1 | 1 (-2.45498) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72099 HOMO: -7.06680 LUMO: 1.86942 factor:1 | 1 (-1.97492) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87846 HOMO: -6.89537 LUMO: 2.17147 factor:1 | 1 (-2.13239) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24074 HOMO: -6.80013 LUMO: 1.78779 factor:1 | 1 (-1.49467) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67765 HOMO: -6.45726 LUMO: 1.58370 factor:1 | 1 (-0.93158) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.46373 HOMO: -6.52529 LUMO: 1.71976 factor:1 | -1 (0.28235) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.84694 HOMO: -7.22462 LUMO: -1.18642 factor:1 | 1 (-0.10087) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.68153 HOMO: -7.18381 LUMO: -0.78641 factor:1 | -1 (0.06455) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79325 HOMO: -6.93346 LUMO: 1.65717 factor:1 | 1 (-1.04718) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41242 HOMO: -6.41644 LUMO: 1.78235 factor:1 | 1 (-0.66635) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60096 HOMO: -6.59876 LUMO: 1.83677 factor:1 | 1 (-1.85489) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65128 HOMO: -6.35658 LUMO: 1.59731 factor:1 | 1 (-1.90521) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83452 HOMO: -6.60692 LUMO: 1.66534 factor:1 | 1 (-2.08845) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99071 HOMO: -6.83006 LUMO: 2.11705 factor:1 | 1 (-2.24464) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41658 HOMO: -6.89264 LUMO: 1.30070 factor:1 | 1 (-1.67051) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53373 HOMO: -6.90081 LUMO: 2.05174 factor:1 | 1 (-0.78766) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85643 HOMO: -6.74842 LUMO: 1.96194 factor:1 | 1 (-1.11036) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.57627 HOMO: -6.58516 LUMO: 1.30887 factor:1 | -1 (0.16980) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.54076 HOMO: -7.00965 LUMO: 2.08167 factor:1 | -1 (0.20531) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.99130 HOMO: -6.86815 LUMO: 2.29664 factor:1 | 1 (-0.24523) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.93740 HOMO: -6.39740 LUMO: 2.02725 factor:1 | 1 (-0.19132) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.92501 HOMO: -5.95929 LUMO: 1.62724 factor:1 | 1 (-0.17894) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.13566 HOMO: -6.71849 LUMO: 1.34696 factor:1 | 1 (-0.38959) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.66629 HOMO: -7.26816 LUMO: 1.74153 factor:1 | -1 (0.07978) | 1 | 1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.35929 HOMO: -6.90897 LUMO: 1.71432 factor:1 | -1 (0.38678) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.25243 HOMO: -6.70489 LUMO: 1.91568 factor:1 | -1 (0.49364) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.93070 HOMO: -6.83278 LUMO: 1.61908 factor:1 | 1 (-0.18463) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.79149 HOMO: -7.17292 LUMO: 1.95378 factor:1 | 1 (-0.04542) | 1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.84969 HOMO: -6.53345 LUMO: 1.74153 factor:1 | 1 (-0.10362) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.73258 HOMO: -6.53073 LUMO: 1.51023 factor:1 | -1 (0.01350) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15091 HOMO: -6.93346 LUMO: 2.22861 factor:1 | 1 (-2.40483) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12285 HOMO: -6.47903 LUMO: 2.05446 factor:1 | 1 (-2.37678) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97115 HOMO: -6.88992 LUMO: 1.57010 factor:1 | 1 (-2.22508) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.17613 HOMO: -6.07358 LUMO: 1.95922 factor:1 | 1 (-2.43006) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.94902 HOMO: -6.75114 LUMO: 2.18780 factor:1 | 1 (-3.20294) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.34767 HOMO: -6.96339 LUMO: 1.70071 factor:1 | 1 (-2.60160) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.43728 HOMO: -7.14843 LUMO: 1.82588 factor:1 | 1 (-2.69121) | 1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11168 HOMO: -6.96339 LUMO: 2.29392 factor:1 | 1 (-1.36560) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67250 HOMO: -6.81645 LUMO: 2.39732 factor:1 | 1 (-1.92643) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.43848 HOMO: -6.48447 LUMO: 1.24084 factor:1 | 1 (-1.69241) | -1 | -1 |
| G: -5245.38038 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49263 HOMO: -7.14843 LUMO: 2.01092 factor:1 | 1 (-1.74656) | 1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.54684 HOMO: -7.20013 LUMO: -0.34286 factor:1 | 1 (-1.80077) | 1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67849 HOMO: -6.97700 LUMO: -0.15238 factor:1 | 1 (-1.93242) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52142 HOMO: -7.07768 LUMO: -0.26123 factor:1 | 1 (-1.77535) | 1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80140 HOMO: -6.99333 LUMO: -0.41361 factor:1 | 1 (-2.05533) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70024 HOMO: -6.84638 LUMO: -0.40273 factor:1 | 1 (-0.95417) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83192 HOMO: -6.83822 LUMO: -0.26939 factor:1 | 1 (-1.08584) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52029 HOMO: -6.75931 LUMO: -0.93879 factor:1 | 1 (-0.77422) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34105 HOMO: -6.79468 LUMO: -0.39729 factor:1 | 1 (-0.59498) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.45071 HOMO: -6.93890 LUMO: 0.43266 factor:1 | 1 (-0.70464) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.78794 HOMO: -7.08040 LUMO: -0.85716 factor:1 | 1 (-1.04187) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.68742 HOMO: -6.70216 LUMO: -1.41499 factor:1 | 1 (-0.94135) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.91456 HOMO: -6.63686 LUMO: -0.52790 factor:1 | 1 (-1.16848) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84590 HOMO: -6.75114 LUMO: -0.13334 factor:1 | 1 (-1.09983) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.05962 HOMO: -6.94435 LUMO: -0.24490 factor:1 | 1 (-1.31355) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.80408 HOMO: -6.74298 LUMO: -0.84627 factor:1 | 1 (-1.05801) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23987 HOMO: -7.15932 LUMO: 0.22041 factor:1 | 1 (-1.49380) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.05562 HOMO: -6.90081 LUMO: -1.16737 factor:1 | 1 (-1.30955) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21969 HOMO: -7.04775 LUMO: -0.84355 factor:1 | 1 (-0.47361) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10208 HOMO: -7.17020 LUMO: -1.31159 factor:1 | 1 (-0.35601) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.20701 HOMO: -7.14571 LUMO: -0.46259 factor:1 | 1 (-0.46093) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64979 HOMO: -7.45048 LUMO: -0.91158 factor:1 | 1 (-0.90372) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.78353 HOMO: -6.87360 LUMO: -0.82995 factor:1 | 1 (-1.03746) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73137 HOMO: -7.43415 LUMO: -0.65307 factor:1 | 1 (-0.98530) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60671 HOMO: -7.47225 LUMO: -0.77280 factor:1 | 1 (-0.86064) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81445 HOMO: -6.86271 LUMO: -0.83811 factor:1 | 1 (-1.06837) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39335 HOMO: -7.53483 LUMO: -0.66124 factor:1 | 1 (-0.64728) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.53472 HOMO: -7.45864 LUMO: -1.08301 factor:1 | -1 (0.21135) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.35706 HOMO: -7.24639 LUMO: -1.19186 factor:1 | -1 (0.38901) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.93816 HOMO: -7.54844 LUMO: -0.96873 factor:1 | 1 (-0.19209) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.68569 HOMO: -7.12666 LUMO: -0.01633 factor:1 | -1 (0.06038) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.64368 HOMO: -6.77291 LUMO: -0.70477 factor:1 | -1 (0.10240) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04044 HOMO: -6.76475 LUMO: -1.15921 factor:1 | 1 (-1.29436) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64696 HOMO: -5.37697 LUMO: -0.56600 factor:1 | 1 (-0.90089) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.29986 HOMO: -6.62053 LUMO: -1.75513 factor:1 | -1 (0.44621) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.61265 HOMO: -6.60420 LUMO: -1.74697 factor:1 | -1 (0.13342) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.45246 HOMO: -6.84366 LUMO: -0.94968 factor:1 | -1 (0.29361) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29674 HOMO: -6.96884 LUMO: -2.11977 factor:1 | 1 (-1.55067) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31354 HOMO: -6.80829 LUMO: 0.56055 factor:1 | 1 (-0.56747) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62323 HOMO: -7.02326 LUMO: 0.11429 factor:1 | 1 (-0.87716) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78274 HOMO: -7.40966 LUMO: 0.18232 factor:1 | 1 (-2.03666) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26678 HOMO: -6.34570 LUMO: 0.41089 factor:1 | 1 (-1.52071) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67155 HOMO: -6.78924 LUMO: 0.49525 factor:1 | 1 (-1.92548) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.47361 HOMO: -6.87632 LUMO: 0.44082 factor:1 | 1 (-2.72753) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.97258 HOMO: -6.69944 LUMO: 1.20546 factor:1 | 1 (-3.22651) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.41486 HOMO: -6.83006 LUMO: 1.28982 factor:1 | 1 (-2.66878) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84614 HOMO: -7.78246 LUMO: 0.20681 factor:1 | 1 (-2.10007) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.61654 HOMO: -6.55794 LUMO: -1.65173 factor:1 | 1 (-0.87047) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66369 HOMO: -6.77564 LUMO: -1.14560 factor:1 | 1 (-0.91762) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56328 HOMO: -7.46680 LUMO: -1.18097 factor:1 | 1 (-0.81721) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53762 HOMO: -6.88176 LUMO: -1.24900 factor:1 | 1 (-0.79155) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53575 HOMO: -7.28177 LUMO: -0.42178 factor:1 | 1 (-0.78967) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58752 HOMO: -7.71715 LUMO: 0.19592 factor:1 | 1 (-1.84145) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37274 HOMO: -7.02326 LUMO: -1.40683 factor:1 | 1 (-1.62667) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51220 HOMO: -7.27088 LUMO: -1.07485 factor:1 | 1 (-1.76613) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98919 HOMO: -7.17020 LUMO: -0.49525 factor:1 | 1 (-2.24312) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74486 HOMO: -7.15932 LUMO: 0.02721 factor:1 | 1 (-1.99879) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64536 HOMO: -7.00693 LUMO: -0.83267 factor:1 | 1 (-2.89929) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.26532 HOMO: -6.86543 LUMO: -0.10340 factor:1 | 1 (-3.51925) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.59260 HOMO: -7.11850 LUMO: -0.08980 factor:1 | 1 (-2.84653) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.83609 HOMO: -6.87087 LUMO: -0.88981 factor:1 | 1 (-3.09002) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62317 HOMO: -7.08857 LUMO: -1.27077 factor:1 | 1 (-1.87710) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63917 HOMO: -6.79468 LUMO: -0.81906 factor:1 | 1 (-1.89310) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39222 HOMO: -6.86815 LUMO: -0.89798 factor:1 | 1 (-1.64615) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54966 HOMO: -6.78652 LUMO: -2.00548 factor:1 | 1 (-2.80359) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50484 HOMO: -6.75114 LUMO: -0.08436 factor:1 | 1 (-2.75877) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.41200 HOMO: -6.55794 LUMO: 0.52790 factor:1 | 1 (-2.66593) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92388 HOMO: -7.17836 LUMO: 0.28300 factor:1 | 1 (-2.17781) | 1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57671 HOMO: -7.35796 LUMO: -0.77552 factor:1 | 1 (-2.83064) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.66000 HOMO: -7.23551 LUMO: -1.17553 factor:1 | 1 (-2.91393) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42986 HOMO: -7.07496 LUMO: -1.14288 factor:1 | 1 (-1.68379) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62543 HOMO: -6.70489 LUMO: -0.83539 factor:1 | 1 (-1.87935) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32967 HOMO: -6.59604 LUMO: -0.89798 factor:1 | 1 (-1.58359) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44734 HOMO: -6.94162 LUMO: -1.22451 factor:1 | 1 (-0.70126) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.23601 HOMO: -6.68040 LUMO: 0.22041 factor:1 | 1 (-0.48994) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.59844 HOMO: -6.88176 LUMO: 0.11157 factor:1 | 1 (-0.85237) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.37090 HOMO: -6.91713 LUMO: 1.27621 factor:1 | 1 (-0.62483) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50024 HOMO: -6.77836 LUMO: 1.01226 factor:1 | 1 (-0.75416) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63207 HOMO: -7.14571 LUMO: 1.48574 factor:1 | 1 (-1.88599) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49715 HOMO: -6.96884 LUMO: 1.48574 factor:1 | 1 (-1.75108) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.24314 HOMO: -7.24367 LUMO: 1.28438 factor:1 | 1 (-0.49707) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.30214 HOMO: -7.10489 LUMO: 1.29526 factor:1 | 1 (-0.55606) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38075 HOMO: -7.07224 LUMO: 1.29254 factor:1 | 1 (-0.63468) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95387 HOMO: -7.12938 LUMO: 0.49253 factor:1 | 1 (-2.20780) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23222 HOMO: -7.33619 LUMO: 1.45581 factor:1 | 1 (-1.48615) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33816 HOMO: -6.87904 LUMO: -0.14422 factor:1 | 1 (-1.59208) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29132 HOMO: -6.81917 LUMO: 0.50341 factor:1 | 1 (-1.54525) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40801 HOMO: -7.27905 LUMO: 0.13606 factor:1 | 1 (-1.66194) | 1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31552 HOMO: -6.87904 LUMO: -0.09796 factor:1 | 1 (-1.56944) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.23875 HOMO: -7.33891 LUMO: 0.03810 factor:1 | 1 (-1.49268) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07535 HOMO: -6.98516 LUMO: 0.98233 factor:1 | 1 (-1.32928) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29380 HOMO: -6.94162 LUMO: 0.86804 factor:1 | 1 (-1.54773) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42379 HOMO: -7.37701 LUMO: 0.05442 factor:1 | 1 (-1.67772) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29187 HOMO: -7.04775 LUMO: 0.43266 factor:1 | 1 (-1.54580) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30063 HOMO: -7.47497 LUMO: 0.31837 factor:1 | 1 (-1.55456) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.10523 HOMO: -6.62053 LUMO: 0.13061 factor:1 | 1 (-1.35915) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.16694 HOMO: -6.44366 LUMO: -0.04354 factor:1 | 1 (-1.42087) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03554 HOMO: -6.40284 LUMO: 0.68301 factor:1 | 1 (-1.28947) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27685 HOMO: -6.73754 LUMO: 0.36735 factor:1 | 1 (-1.53078) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27927 HOMO: -6.85455 LUMO: 0.23946 factor:1 | 1 (-1.53320) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.16993 HOMO: -6.93346 LUMO: 0.24762 factor:1 | 1 (-1.42386) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22147 HOMO: -6.85455 LUMO: 0.17687 factor:1 | 1 (-1.47540) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11491 HOMO: -6.62325 LUMO: 0.69933 factor:1 | 1 (-1.36884) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32588 HOMO: -6.43005 LUMO: 0.50069 factor:1 | 1 (-1.57981) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33935 HOMO: -6.56883 LUMO: 0.22858 factor:1 | 1 (-1.59328) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27737 HOMO: -6.78380 LUMO: 0.54967 factor:1 | 1 (-1.53129) | -1 | -1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08101 HOMO: -7.35524 LUMO: 0.00272 factor:1 | 1 (-1.33494) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35255 HOMO: -7.27360 LUMO: 0.08436 factor:1 | 1 (-1.60648) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.80380 HOMO: -7.44504 LUMO: -0.96056 factor:1 | 1 (-2.05773) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.21978 HOMO: -7.27360 LUMO: 0.29933 factor:1 | 1 (-2.47371) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.16122 HOMO: -7.09129 LUMO: 0.41089 factor:1 | 1 (-2.41515) | 1 | 1 |
| G: -5245.38038 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42559 HOMO: -6.93618 LUMO: 0.36463 factor:1 | 1 (-1.67951) | -1 | -1 |
| G: -5245.38038 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18664 HOMO: -7.65728 LUMO: 0.20136 factor:1 | 1 (-1.44057) | 1 | 1 |
| G: -5245.38038 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84664 HOMO: -6.90353 LUMO: -0.92791 factor:1 | 1 (-1.10056) | -1 | -1 |
| G: -5245.38038 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.02064 HOMO: -6.82462 LUMO: -1.18370 factor:1 | 1 (-2.27457) | -1 | -1 |
| G: -5245.38038 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.98888 HOMO: -7.09129 LUMO: -0.13334 factor:1 | 1 (-3.24281) | 1 | 1 |
| G: -5245.38038 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12742 HOMO: -7.40966 LUMO: -1.06941 factor:1 | 1 (-2.38135) | 1 | 1 |
| G: -5245.38038 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.58460 HOMO: -7.24367 LUMO: -1.00954 factor:1 | 1 (-2.83853) | 1 | 1 |
| G: -5245.38038 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54240 HOMO: -7.51851 LUMO: 0.09796 factor:1 | 1 (-2.79632) | 1 | 1 |
| G: -5245.38038 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52938 HOMO: -7.48857 LUMO: -0.07619 factor:1 | 1 (-0.78331) | 1 | 1 |
| G: -5245.38038 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52102 HOMO: -6.53345 LUMO: 1.09390 factor:1 | 1 (-0.77495) | -1 | -1 |
| G: -5245.38038 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31392 HOMO: -7.21918 LUMO: 0.08436 factor:1 | 1 (-0.56785) | 1 | 1 |
| G: -5245.38038 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47996 HOMO: -7.38789 LUMO: 1.02587 factor:1 | 1 (-0.73389) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34973 HOMO: -6.83550 LUMO: -0.67484 factor:1 | 1 (-0.60366) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96324 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-1.21717) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89611 HOMO: -6.79740 LUMO: 1.91296 factor:1 | 1 (-1.15003) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72955 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-0.98347) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84813 HOMO: -6.62597 LUMO: -0.44082 factor:1 | 1 (-1.10206) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90816 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-1.16209) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90307 HOMO: -6.51168 LUMO: -0.23130 factor:1 | 1 (-1.15700) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.82280 HOMO: -7.14027 LUMO: 0.49797 factor:1 | 1 (-1.07673) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89001 HOMO: -7.55660 LUMO: 0.24762 factor:1 | 1 (-1.14394) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.07627 HOMO: -6.88992 LUMO: -0.64763 factor:1 | 1 (-1.33020) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04030 HOMO: -6.72665 LUMO: -0.45987 factor:1 | 1 (-1.29423) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89747 HOMO: -6.72121 LUMO: -0.58232 factor:1 | 1 (-1.15140) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44074 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-1.69467) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01235 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-1.26628) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54309 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-0.79702) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.28453 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-0.53846) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.53180 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-0.78573) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.22690 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-0.48083) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.45806 HOMO: -6.79740 LUMO: -0.55511 factor:1 | 1 (-0.71199) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.03244 HOMO: -6.79740 LUMO: -0.67756 factor:1 | 1 (-1.28636) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26542 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-1.51935) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.99206 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-0.24599) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.04221 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-0.29614) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39759 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-0.65152) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.99048 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-0.24441) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19022 HOMO: -6.59332 LUMO: -0.27211 factor:1 | 1 (-0.44414) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.61466 HOMO: -6.57427 LUMO: -0.16871 factor:1 | 1 (-0.86859) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.30614 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-0.56006) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39417 HOMO: -6.72121 LUMO: 2.00004 factor:1 | 1 (-0.64809) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64228 HOMO: -6.61509 LUMO: 1.55921 factor:1 | 1 (-0.89621) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.80089 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-1.05482) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64984 HOMO: -6.66135 LUMO: 2.02181 factor:1 | 1 (-0.90377) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81877 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-1.07270) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44772 HOMO: -6.66679 LUMO: 1.98371 factor:1 | 1 (-0.70165) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90751 HOMO: -6.67495 LUMO: 2.04085 factor:1 | 1 (-1.16144) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.04581 HOMO: -6.89809 LUMO: 1.95106 factor:1 | 1 (-2.29974) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78717 HOMO: -6.50352 LUMO: 1.88847 factor:1 | 1 (-2.04110) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87223 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-2.12616) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.07899 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-2.33291) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54222 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-0.79615) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50372 HOMO: -6.65591 LUMO: 2.20684 factor:1 | 1 (-0.75765) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51673 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-0.77065) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29242 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-0.54635) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.20382 HOMO: -6.53617 LUMO: 1.75241 factor:1 | 1 (-0.45775) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19120 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-0.44512) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.94930 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-1.20323) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90272 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-1.15665) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.82302 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-1.07695) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.80176 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-1.05569) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00430 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-1.25823) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37271 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-1.62664) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44025 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-1.69418) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53764 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-1.79157) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58439 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-1.83832) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63582 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-1.88975) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.93374 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-1.18767) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.69858 HOMO: -6.90897 LUMO: 1.91296 factor:1 | 1 (-0.95251) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79096 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-1.04489) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.90403 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-1.15795) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.72035 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-0.97428) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81861 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-1.07254) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65597 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-0.90989) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65757 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-0.91150) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73959 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-0.99351) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.09197 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-2.34589) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08029 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-2.33422) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.10957 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-2.36350) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.07224 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-2.32617) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.04410 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-2.29803) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.01945 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-2.27338) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99251 HOMO: -6.75387 LUMO: 1.72248 factor:1 | 1 (-2.24644) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92998 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-2.18390) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.07471 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-2.32864) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70840 HOMO: -6.80557 LUMO: 2.02725 factor:1 | 1 (-0.96233) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.91265 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-1.16658) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84895 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-1.10288) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01273 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-1.26666) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89777 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-1.15169) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73393 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-0.98785) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75755 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-1.01147) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83246 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-1.08639) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00827 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-1.26220) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66094 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-1.91487) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70162 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-1.95555) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60015 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-1.85407) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.61313 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-1.86705) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79513 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-1.04905) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44667 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-1.70060) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00528 HOMO: -6.64230 LUMO: 2.16058 factor:1 | 1 (-1.25921) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37380 HOMO: -6.58788 LUMO: 2.10616 factor:1 | 1 (-1.62773) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31639 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-1.57031) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.78756 HOMO: -6.31304 LUMO: 2.31841 factor:1 | 1 (-1.04149) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12452 HOMO: -6.94979 LUMO: 2.07895 factor:1 | 1 (-1.37845) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.68201 HOMO: -6.88992 LUMO: 2.28031 factor:1 | 1 (-0.93594) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.98661 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-1.24054) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73472 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-0.98864) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96732 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-1.22125) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41740 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-1.67132) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31701 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-1.57094) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39984 HOMO: -6.31304 LUMO: 2.18507 factor:1 | 1 (-1.65377) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29777 HOMO: -6.18243 LUMO: 2.01636 factor:1 | 1 (-1.55170) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51563 HOMO: -6.99877 LUMO: 2.14970 factor:1 | 1 (-1.76956) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.47269 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-1.72662) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68252 HOMO: -6.36202 LUMO: 2.17419 factor:1 | 1 (-1.93644) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63163 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-1.88556) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63354 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-1.88746) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75947 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-2.01340) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.93701 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-1.19093) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00607 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-1.26000) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21845 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-1.47238) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00735 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-1.26127) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84366 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-2.09759) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74665 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-2.00058) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73152 HOMO: -6.44094 LUMO: 1.74425 factor:1 | 1 (-1.98545) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76725 HOMO: -6.51985 LUMO: 1.84221 factor:1 | 1 (-2.02118) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.69685 HOMO: -6.63414 LUMO: -0.24762 factor:1 | 1 (-2.95078) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62738 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-2.88130) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.25122 HOMO: -7.19741 LUMO: 0.58232 factor:1 | 1 (-3.50515) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.37164 HOMO: -6.77019 LUMO: -0.56872 factor:1 | 1 (-2.62557) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.22057 HOMO: -7.46136 LUMO: 0.28844 factor:1 | 1 (-2.47449) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.92170 HOMO: -6.60420 LUMO: -0.54151 factor:1 | 1 (-3.17562) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.88520 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-3.13913) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.43213 HOMO: -6.81645 LUMO: -0.57144 factor:1 | 1 (-2.68606) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59002 HOMO: -7.48041 LUMO: 0.28572 factor:1 | 1 (-1.84395) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.92066 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-3.17459) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.98317 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-3.23709) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.77981 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-3.03374) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.05160 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-3.30553) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93498 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-2.18891) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84864 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-2.10257) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.09912 HOMO: -6.50896 LUMO: -0.25034 factor:1 | 1 (-2.35305) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.22125 HOMO: -7.17564 LUMO: -0.68573 factor:1 | 1 (-2.47517) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.23619 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-2.49011) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97942 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-2.23335) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87931 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-2.13324) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88524 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-2.13917) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98886 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-2.24279) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81400 HOMO: -6.62325 LUMO: 2.02725 factor:1 | 1 (-2.06793) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14454 HOMO: -6.63414 LUMO: 1.91296 factor:1 | 1 (-2.39847) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.51475 HOMO: -6.83278 LUMO: 1.65717 factor:1 | -1 (0.23132) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.68789 HOMO: -6.66407 LUMO: 1.95650 factor:1 | -1 (0.05818) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.60221 HOMO: -6.61237 LUMO: 2.11432 factor:1 | -1 (0.14387) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.08347 HOMO: -6.62053 LUMO: 2.09256 factor:1 | 1 (-0.33739) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.00376 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-0.25769) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.86999 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-0.12392) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10178 HOMO: -6.85183 LUMO: 2.12793 factor:1 | 1 (-0.35571) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82619 HOMO: -6.81101 LUMO: 1.83949 factor:1 | 1 (-2.08012) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63413 HOMO: -6.98788 LUMO: 2.16058 factor:1 | 1 (-1.88806) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56137 HOMO: -6.62869 LUMO: 2.00820 factor:1 | 1 (-1.81530) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17294 HOMO: -6.34025 LUMO: 2.25855 factor:1 | 1 (-0.42687) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.10553 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-0.35946) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39433 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-0.64826) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.26771 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-0.52164) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.09767 HOMO: -6.83278 LUMO: 1.53744 factor:1 | 1 (-0.35160) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87634 HOMO: -6.41917 LUMO: 1.82316 factor:1 | 1 (-2.13027) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.18980 HOMO: -6.56339 LUMO: 1.63813 factor:1 | 1 (-1.44373) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.08865 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-1.34258) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37016 HOMO: -6.63141 LUMO: 1.92112 factor:1 | 1 (-1.62408) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.85965 HOMO: -6.83822 LUMO: 1.88847 factor:1 | 1 (-3.11358) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.66291 HOMO: -6.84638 LUMO: 1.90480 factor:1 | 1 (-3.91683) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.80338 HOMO: -6.82462 LUMO: 1.70888 factor:1 | 1 (-3.05731) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01596 HOMO: -6.82734 LUMO: 2.12521 factor:1 | 1 (-3.26988) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97751 HOMO: -6.94435 LUMO: 1.87214 factor:1 | 1 (-2.23144) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97806 HOMO: -6.98516 LUMO: 2.51433 factor:1 | 1 (-2.23199) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48483 HOMO: -6.74026 LUMO: 2.15514 factor:1 | 1 (-1.73875) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69588 HOMO: -6.93618 LUMO: 2.54426 factor:1 | 1 (-1.94980) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50344 HOMO: -6.28583 LUMO: 2.53610 factor:1 | 1 (-1.75737) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63901 HOMO: -6.56883 LUMO: 1.94834 factor:1 | 1 (-0.89294) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.96280 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-1.21673) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76702 HOMO: -6.19059 LUMO: 1.99732 factor:1 | 1 (-1.02094) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59979 HOMO: -6.78108 LUMO: 2.03813 factor:1 | 1 (-1.85372) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88524 HOMO: -6.82189 LUMO: 1.77418 factor:1 | 1 (-2.13917) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31709 HOMO: -6.45454 LUMO: 1.78779 factor:1 | 1 (-2.57101) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.30549 HOMO: -6.84366 LUMO: 1.77690 factor:1 | 1 (-2.55942) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.84761 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-2.10154) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95153 HOMO: -6.76475 LUMO: 2.40277 factor:1 | 1 (-2.20546) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79063 HOMO: -6.65863 LUMO: 1.86670 factor:1 | 1 (-2.04455) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79512 HOMO: -6.50080 LUMO: 1.93201 factor:1 | 1 (-2.04904) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.26763 HOMO: -6.34842 LUMO: 1.70888 factor:1 | 1 (-0.52156) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.22358 HOMO: -6.60692 LUMO: 2.20140 factor:1 | 1 (-0.47751) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43272 HOMO: -6.74026 LUMO: 2.14970 factor:1 | 1 (-0.68665) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43700 HOMO: -6.63686 LUMO: 2.17419 factor:1 | 1 (-0.69092) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36543 HOMO: -6.81917 LUMO: 2.10072 factor:1 | 1 (-0.61936) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43765 HOMO: -6.92802 LUMO: 2.04358 factor:1 | 1 (-0.69158) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49716 HOMO: -6.56067 LUMO: -0.47620 factor:1 | 1 (-0.75109) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46102 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-0.71495) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52549 HOMO: -6.78380 LUMO: -0.64763 factor:1 | 1 (-0.77942) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24841 HOMO: -6.51985 LUMO: -0.24490 factor:1 | 1 (-1.50234) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26833 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-1.52226) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30844 HOMO: -7.10489 LUMO: -0.62586 factor:1 | 1 (-1.56237) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91229 HOMO: -7.18108 LUMO: 0.48980 factor:1 | 1 (-2.16622) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78611 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-2.04004) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.23958 HOMO: -6.70761 LUMO: -0.54423 factor:1 | 1 (-3.49351) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50318 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-2.75711) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.54561 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-2.79953) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56057 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-2.81450) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.97973 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-1.23366) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25641 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-1.51034) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.14675 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-1.40068) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.91940 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-1.17333) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37655 HOMO: -6.66951 LUMO: -0.40817 factor:1 | 1 (-1.63048) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.20545 HOMO: -6.60420 LUMO: -0.19320 factor:1 | 1 (-1.45937) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09540 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-1.34933) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.16686 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-1.42079) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41184 HOMO: -7.27088 LUMO: 0.53334 factor:1 | 1 (-1.66577) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77466 HOMO: -7.20013 LUMO: 0.59049 factor:1 | 1 (-1.02859) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11573 HOMO: -6.60148 LUMO: -0.20953 factor:1 | 1 (-1.36966) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09238 HOMO: -6.69400 LUMO: -0.51974 factor:1 | 1 (-1.34631) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.99521 HOMO: -7.40422 LUMO: -0.98777 factor:1 | 1 (-1.24914) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.04773 HOMO: -6.88176 LUMO: -0.71022 factor:1 | 1 (-1.30166) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38632 HOMO: -6.86271 LUMO: -0.59321 factor:1 | 1 (-1.64025) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.94743 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-1.20136) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.93350 HOMO: -6.71033 LUMO: 1.57010 factor:1 | 1 (-1.18742) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.60605 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-1.85998) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50869 HOMO: -6.67495 LUMO: 2.03813 factor:1 | 1 (-1.76262) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50355 HOMO: -6.54434 LUMO: 1.83677 factor:1 | 1 (-1.75747) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71022 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-1.96415) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30022 HOMO: -6.76747 LUMO: 1.87759 factor:1 | 1 (-1.55415) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.93857 HOMO: -6.58243 LUMO: 1.61364 factor:1 | 1 (-3.19249) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.14911 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-2.40304) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31330 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-2.56723) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52697 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-2.78089) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08742 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-2.34135) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.22644 HOMO: -6.83278 LUMO: 1.91296 factor:1 | 1 (-2.48037) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15814 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-2.41207) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.32411 HOMO: -6.50080 LUMO: 1.73337 factor:1 | 1 (-2.57803) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.01093 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-2.26486) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.05724 HOMO: -6.63686 LUMO: 2.20140 factor:1 | 1 (-2.31117) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.34038 HOMO: -6.57427 LUMO: 1.87214 factor:1 | 1 (-2.59431) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93158 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-2.18551) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.11967 HOMO: -6.63958 LUMO: 2.04902 factor:1 | 1 (-2.37359) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97757 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-2.23150) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.36294 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-2.61686) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45864 HOMO: -6.72938 LUMO: 2.28304 factor:1 | 1 (-2.71257) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52893 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-2.78285) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52054 HOMO: -6.95523 LUMO: 2.33474 factor:1 | 1 (-2.77447) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40335 HOMO: -6.59876 LUMO: 2.30480 factor:1 | 1 (-1.65728) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30167 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-1.55559) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.29196 HOMO: -7.06408 LUMO: 1.99187 factor:1 | 1 (-3.54589) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.30382 HOMO: -6.95795 LUMO: 1.88847 factor:1 | 1 (-3.55775) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.05560 HOMO: -6.85455 LUMO: 1.63813 factor:1 | 1 (-3.30953) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.09294 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-3.34686) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81346 HOMO: -6.91441 LUMO: 1.68983 factor:1 | 1 (-2.06739) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94429 HOMO: -6.89809 LUMO: 2.23678 factor:1 | 1 (-2.19822) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97330 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-2.22722) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85389 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-2.10782) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69324 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-1.94717) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79860 HOMO: -6.94979 LUMO: 2.28031 factor:1 | 1 (-2.05253) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88219 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-2.13612) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92998 HOMO: -6.87360 LUMO: 2.40277 factor:1 | 1 (-2.18390) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.81718 HOMO: -6.92802 LUMO: 1.89663 factor:1 | 1 (-3.07110) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.03980 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-2.29373) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.14584 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-3.39976) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.55833 HOMO: -6.54978 LUMO: 1.93201 factor:1 | 1 (-3.81226) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.89121 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-1.14514) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.80680 HOMO: -6.55794 LUMO: 1.89663 factor:1 | 1 (-1.06073) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35505 HOMO: -6.07630 LUMO: 1.94289 factor:1 | 1 (-1.60898) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01182 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-3.26575) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.14679 HOMO: -6.63958 LUMO: -0.61770 factor:1 | 1 (-3.40072) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.86684 HOMO: -6.81101 LUMO: -0.57960 factor:1 | 1 (-3.12077) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.89723 HOMO: -6.74298 LUMO: -0.57960 factor:1 | 1 (-3.15116) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66012 HOMO: -6.63686 LUMO: -0.42994 factor:1 | 1 (-1.91405) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72777 HOMO: -6.60965 LUMO: -0.41089 factor:1 | 1 (-1.98170) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.47535 HOMO: -6.60692 LUMO: -0.80274 factor:1 | 1 (-2.72927) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88252 HOMO: -6.58788 LUMO: -0.78097 factor:1 | 1 (-2.13645) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65324 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-1.90716) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48727 HOMO: -6.63141 LUMO: -0.40545 factor:1 | 1 (-2.74119) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56463 HOMO: -6.62053 LUMO: -0.83811 factor:1 | 1 (-2.81856) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88995 HOMO: -6.59604 LUMO: -0.35375 factor:1 | 1 (-2.14388) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79925 HOMO: -6.34297 LUMO: -0.39729 factor:1 | 1 (-2.05318) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.96072 HOMO: -6.67223 LUMO: 1.97827 factor:1 | 1 (-2.21465) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70418 HOMO: -6.40012 LUMO: 1.89935 factor:1 | 1 (-1.95810) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73797 HOMO: -6.74842 LUMO: 1.97283 factor:1 | 1 (-1.99190) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73463 HOMO: -6.76747 LUMO: 2.17147 factor:1 | 1 (-1.98855) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78453 HOMO: -6.72121 LUMO: 1.55649 factor:1 | 1 (-2.03846) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79313 HOMO: -6.97700 LUMO: 2.04085 factor:1 | 1 (-2.04706) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78954 HOMO: -7.06680 LUMO: 2.04085 factor:1 | 1 (-2.04347) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.78742 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-2.04134) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68439 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-1.93832) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55900 HOMO: -6.72665 LUMO: 2.20140 factor:1 | 1 (-1.81293) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82578 HOMO: -6.77291 LUMO: 2.34562 factor:1 | 1 (-2.07971) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59427 HOMO: -6.73754 LUMO: 2.00276 factor:1 | 1 (-1.84820) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73101 HOMO: -7.04231 LUMO: 1.92112 factor:1 | 1 (-1.98493) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87144 HOMO: -6.83822 LUMO: 1.72248 factor:1 | 1 (-2.12537) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86592 HOMO: -6.57971 LUMO: 2.16603 factor:1 | 1 (-2.11985) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73650 HOMO: -6.80013 LUMO: 1.88575 factor:1 | 1 (-1.99043) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81506 HOMO: -6.93618 LUMO: 2.18235 factor:1 | 1 (-2.06899) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68102 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-1.93495) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.90094 HOMO: -7.06952 LUMO: 2.18507 factor:1 | 1 (-2.15487) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69351 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-1.94744) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81789 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-2.07182) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.39499 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-2.64892) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.32215 HOMO: -7.17292 LUMO: 1.90752 factor:1 | 1 (-2.57607) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.23208 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-2.48601) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.42718 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-2.68111) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.32062 HOMO: -6.85727 LUMO: 2.13609 factor:1 | 1 (-2.57455) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.41116 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-2.66508) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.44819 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-2.70212) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.33352 HOMO: -6.67223 LUMO: 2.07351 factor:1 | 1 (-2.58745) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.36691 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-2.62084) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.96847 HOMO: -6.90897 LUMO: 2.28848 factor:1 | 1 (-3.22240) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.84722 HOMO: -7.04231 LUMO: 1.70071 factor:1 | 1 (-3.10115) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.58629 HOMO: -6.69944 LUMO: 1.94834 factor:1 | 1 (-2.84022) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62444 HOMO: -6.56067 LUMO: 2.20956 factor:1 | 1 (-2.87837) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71000 HOMO: -6.65046 LUMO: 2.06807 factor:1 | 1 (-1.96393) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48896 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-1.74289) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.94850 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-3.20243) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52989 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-1.78382) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.10162 HOMO: -6.85183 LUMO: 2.16058 factor:1 | 1 (-3.35554) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52637 HOMO: -6.54706 LUMO: 1.92384 factor:1 | 1 (-2.78030) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.07142 HOMO: -6.84366 LUMO: 2.48984 factor:1 | 1 (-2.32535) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79718 HOMO: -6.77291 LUMO: 2.46263 factor:1 | 1 (-2.05111) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08731 HOMO: -7.01782 LUMO: 2.31025 factor:1 | 1 (-2.34124) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92252 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-2.17645) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77446 HOMO: -6.64230 LUMO: 1.97283 factor:1 | 1 (-2.02839) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77060 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-2.02453) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69454 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-1.94847) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.97392 HOMO: -7.17020 LUMO: 2.06807 factor:1 | 1 (-2.22785) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77416 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-2.02809) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.59155 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-1.84548) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31230 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-2.56622) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.67459 HOMO: -6.92802 LUMO: 1.99187 factor:1 | 1 (-2.92852) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.57462 HOMO: -6.69672 LUMO: 2.36739 factor:1 | 1 (-1.82855) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33135 HOMO: -7.13755 LUMO: 2.00276 factor:1 | 1 (-1.58528) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.21645 HOMO: -6.92530 LUMO: 2.25582 factor:1 | 1 (-3.47038) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.56626 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-2.82019) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.61080 HOMO: -6.87904 LUMO: 1.60003 factor:1 | 1 (-2.86473) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17731 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-1.43124) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.34769 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-3.60162) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.50649 HOMO: -6.74298 LUMO: 1.47486 factor:1 | 1 (-3.76042) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11514.18289 HOMO: -6.77019 LUMO: 1.90480 factor:1 | 1 (-4.43682) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.78378 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-4.03771) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.91802 HOMO: -6.73482 LUMO: 2.08711 factor:1 | 1 (-3.17195) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.80463 HOMO: -6.46543 LUMO: 1.73881 factor:1 | 1 (-3.05856) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.50307 HOMO: -6.96067 LUMO: 2.26127 factor:1 | 1 (-3.75699) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.80558 HOMO: -6.67767 LUMO: 2.10616 factor:1 | 1 (-3.05951) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79340 HOMO: -6.28855 LUMO: 2.35923 factor:1 | 1 (-2.04733) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66888 HOMO: -6.80285 LUMO: 1.62724 factor:1 | 1 (-1.92281) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.74172 HOMO: -6.85455 LUMO: 2.23133 factor:1 | 1 (-2.99565) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87319 HOMO: -6.51713 LUMO: 2.33474 factor:1 | 1 (-2.12711) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.02809 HOMO: -6.88176 LUMO: 2.15242 factor:1 | 1 (-3.28202) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68679 HOMO: -6.54434 LUMO: 2.32113 factor:1 | 1 (-1.94072) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.59483 HOMO: -6.62597 LUMO: 2.24222 factor:1 | 1 (-2.84876) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70039 HOMO: -6.74570 LUMO: 2.19868 factor:1 | 1 (-1.95432) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65589 HOMO: -6.62869 LUMO: 1.98915 factor:1 | 1 (-2.90982) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.70985 HOMO: -6.64502 LUMO: 2.13881 factor:1 | 1 (-2.96378) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.76235 HOMO: -6.95795 LUMO: 1.82316 factor:1 | 1 (-3.01627) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.69900 HOMO: -6.77291 LUMO: 1.36329 factor:1 | 1 (-2.95293) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.37833 HOMO: -6.45726 LUMO: 1.73064 factor:1 | 1 (-3.63226) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55962 HOMO: -6.49264 LUMO: 1.77418 factor:1 | 1 (-2.81355) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.46615 HOMO: -6.60420 LUMO: 2.20956 factor:1 | 1 (-2.72008) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.33566 HOMO: -6.56067 LUMO: 2.05718 factor:1 | 1 (-3.58959) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65611 HOMO: -6.62597 LUMO: 1.70343 factor:1 | 1 (-2.91004) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.70136 HOMO: -6.69400 LUMO: 2.16875 factor:1 | 1 (-2.95529) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65102 HOMO: -6.63958 LUMO: 2.11977 factor:1 | 1 (-2.90495) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.70436 HOMO: -6.92802 LUMO: 1.82044 factor:1 | 1 (-2.95829) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.35229 HOMO: -6.56339 LUMO: 2.30480 factor:1 | 1 (-3.60622) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.34114 HOMO: -6.63958 LUMO: 1.91024 factor:1 | 1 (-2.59507) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.06325 HOMO: -6.93074 LUMO: 2.05446 factor:1 | 1 (-3.31718) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.44601 HOMO: -6.61509 LUMO: 2.03813 factor:1 | 1 (-2.69994) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49956 HOMO: -6.61237 LUMO: 1.91296 factor:1 | 1 (-2.75349) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.28479 HOMO: -6.86815 LUMO: 1.95378 factor:1 | 1 (-2.53871) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.21468 HOMO: -6.63686 LUMO: 1.70888 factor:1 | 1 (-3.46861) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48593 HOMO: -6.57971 LUMO: 2.20140 factor:1 | 1 (-2.73986) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.32603 HOMO: -6.41100 LUMO: 1.96738 factor:1 | 1 (-3.57996) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.83526 HOMO: -6.90081 LUMO: 1.65989 factor:1 | 1 (-4.08919) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.09318 HOMO: -6.68312 LUMO: 1.97827 factor:1 | 1 (-3.34711) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.98681 HOMO: -6.65318 LUMO: 2.10888 factor:1 | 1 (-3.24074) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.57052 HOMO: -6.62053 LUMO: 2.28848 factor:1 | 1 (-3.82445) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.74239 HOMO: -6.65863 LUMO: 2.29664 factor:1 | 1 (-3.99632) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.10045 HOMO: -6.63958 LUMO: 2.07623 factor:1 | 1 (-3.35437) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.69730 HOMO: -6.58243 LUMO: 2.20684 factor:1 | 1 (-3.95123) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.50566 HOMO: -6.59332 LUMO: 2.05174 factor:1 | 1 (-2.75959) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.14649 HOMO: -6.95251 LUMO: 2.20140 factor:1 | 1 (-3.40042) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.17993 HOMO: -6.84638 LUMO: 2.39732 factor:1 | 1 (-3.43386) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.49859 HOMO: -6.86815 LUMO: 2.47896 factor:1 | 1 (-2.75251) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.33112 HOMO: -7.00693 LUMO: 2.43270 factor:1 | 1 (-3.58505) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64079 HOMO: -6.58788 LUMO: 2.30208 factor:1 | 1 (-2.89472) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.91454 HOMO: -6.63958 LUMO: 2.28031 factor:1 | 1 (-3.16847) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.11343 HOMO: -6.74570 LUMO: 2.28304 factor:1 | 1 (-3.36735) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.43189 HOMO: -6.78380 LUMO: 2.16331 factor:1 | 1 (-2.68582) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.08744 HOMO: -6.52529 LUMO: 2.05718 factor:1 | 1 (-3.34137) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.62685 HOMO: -6.41644 LUMO: 1.65445 factor:1 | 1 (-3.88078) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.69736 HOMO: -6.34570 LUMO: 1.22451 factor:1 | 1 (-3.95128) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.13941 HOMO: -6.14433 LUMO: 1.85582 factor:1 | 1 (-3.39334) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.25950 HOMO: -6.62053 LUMO: 1.92112 factor:1 | 1 (-3.51343) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65791 HOMO: -6.63414 LUMO: 1.61908 factor:1 | 1 (-2.91184) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.84987 HOMO: -6.75931 LUMO: 1.87214 factor:1 | 1 (-1.10380) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75322 HOMO: -6.55794 LUMO: 1.77418 factor:1 | 1 (-1.00715) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.17141 HOMO: -6.52801 LUMO: 1.82044 factor:1 | 1 (-3.42534) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.77600 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-1.02992) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.75491 HOMO: -6.93890 LUMO: 1.81228 factor:1 | 1 (-1.00883) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70995 HOMO: -6.85455 LUMO: 1.75513 factor:1 | 1 (-0.96388) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83284 HOMO: -6.86815 LUMO: 1.64629 factor:1 | 1 (-1.08677) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.76582 HOMO: -6.98516 LUMO: 1.84765 factor:1 | 1 (-1.01975) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.84324 HOMO: -6.04637 LUMO: 1.94017 factor:1 | 1 (-3.09717) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.61935 HOMO: -6.86271 LUMO: 2.11977 factor:1 | 1 (-2.87328) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64161 HOMO: -6.72938 LUMO: 2.11160 factor:1 | 1 (-2.89554) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68349 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-2.93741) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.78106 HOMO: -6.18515 LUMO: 2.04630 factor:1 | 1 (-1.03499) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.52701 HOMO: -6.60965 LUMO: 2.17147 factor:1 | 1 (-3.78094) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.00654 HOMO: -6.87360 LUMO: 2.35378 factor:1 | 1 (-3.26047) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.98702 HOMO: -6.72938 LUMO: 2.20140 factor:1 | 1 (-1.24095) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99455 HOMO: -6.88448 LUMO: 2.54154 factor:1 | 1 (-2.24848) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.75366 HOMO: -6.87087 LUMO: 2.16058 factor:1 | 1 (-3.00759) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98168 HOMO: -7.11306 LUMO: 2.04085 factor:1 | 1 (-2.23561) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.23261 HOMO: -6.66951 LUMO: 1.68438 factor:1 | 1 (-3.48654) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.44843 HOMO: -7.08312 LUMO: 2.19324 factor:1 | 1 (-3.70235) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.22654 HOMO: -6.69128 LUMO: 2.13881 factor:1 | 1 (-3.48047) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.06657 HOMO: -6.80285 LUMO: 2.16603 factor:1 | 1 (-3.32050) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.01405 HOMO: -6.82189 LUMO: 2.46807 factor:1 | 1 (-3.26798) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.24205 HOMO: -6.78652 LUMO: 2.12521 factor:1 | 1 (-1.49597) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46833 HOMO: -6.47903 LUMO: 1.70071 factor:1 | 1 (-1.72226) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26455 HOMO: -6.37019 LUMO: 1.24356 factor:1 | 1 (-1.51848) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.92338 HOMO: -6.69400 LUMO: 1.67350 factor:1 | 1 (-3.17731) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.78115 HOMO: -7.51851 LUMO: 0.27756 factor:1 | 1 (-3.03508) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.85851 HOMO: -6.95795 LUMO: -0.72110 factor:1 | 1 (-3.11244) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67861 HOMO: -6.88720 LUMO: -0.67484 factor:1 | 1 (-0.93253) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.85545 HOMO: -6.83550 LUMO: -0.57144 factor:1 | 1 (-1.10938) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.81638 HOMO: -6.80285 LUMO: -0.57144 factor:1 | 1 (-1.07031) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62293 HOMO: -6.76475 LUMO: -0.53062 factor:1 | 1 (-0.87686) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98296 HOMO: -6.66951 LUMO: 1.74969 factor:1 | 1 (-2.23688) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.39431 HOMO: -6.53345 LUMO: 1.89935 factor:1 | 1 (-2.64824) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45752 HOMO: -6.65046 LUMO: 2.01364 factor:1 | 1 (-2.71145) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72224 HOMO: -6.64230 LUMO: 2.11977 factor:1 | 1 (-1.97617) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75378 HOMO: -6.44910 LUMO: 2.13337 factor:1 | 1 (-2.00771) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71182 HOMO: -7.05591 LUMO: 1.98915 factor:1 | 1 (-1.96575) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.84006 HOMO: -7.02326 LUMO: 2.49256 factor:1 | 1 (-3.09399) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.76839 HOMO: -6.32937 LUMO: 2.51161 factor:1 | 1 (-3.02231) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.46875 HOMO: -6.96067 LUMO: 2.20140 factor:1 | 1 (-3.72268) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.76362 HOMO: -6.97972 LUMO: 2.55243 factor:1 | 1 (-3.01755) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62506 HOMO: -6.72665 LUMO: 2.46535 factor:1 | 1 (-2.87899) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52776 HOMO: -6.41917 LUMO: 2.35106 factor:1 | 1 (-1.78169) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45848 HOMO: -6.75114 LUMO: 2.32929 factor:1 | 1 (-1.71241) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48463 HOMO: -6.91713 LUMO: 2.27215 factor:1 | 1 (-1.73856) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.27651 HOMO: -6.54978 LUMO: 2.00276 factor:1 | 1 (-2.53044) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.26563 HOMO: -6.62325 LUMO: 2.05990 factor:1 | 1 (-2.51956) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12280 HOMO: -6.86271 LUMO: 2.14970 factor:1 | 1 (-2.37672) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.15052 HOMO: -6.77564 LUMO: 2.25855 factor:1 | 1 (-2.40445) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.77897 HOMO: -6.71305 LUMO: 1.94561 factor:1 | 1 (-3.03290) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64384 HOMO: -6.75659 LUMO: 1.94561 factor:1 | 1 (-2.89777) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.96151 HOMO: -6.94979 LUMO: 2.33474 factor:1 | 1 (-3.21543) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.76640 HOMO: -6.85727 LUMO: 2.50345 factor:1 | 1 (-3.02033) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53514 HOMO: -6.87360 LUMO: 2.43270 factor:1 | 1 (-1.78907) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46771 HOMO: -6.57427 LUMO: 2.46807 factor:1 | 1 (-1.72164) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66459 HOMO: -7.16204 LUMO: 2.15242 factor:1 | 1 (-0.91852) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70086 HOMO: -6.62869 LUMO: 2.11432 factor:1 | 1 (-0.95479) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.40557 HOMO: -7.05591 LUMO: 2.26671 factor:1 | 1 (-3.65950) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.22754 HOMO: -7.13483 LUMO: 1.47758 factor:1 | 1 (-1.48147) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25916 HOMO: -6.72938 LUMO: 1.57282 factor:1 | 1 (-1.51309) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.19094 HOMO: -6.17426 LUMO: 1.81228 factor:1 | 1 (-1.44487) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72460 HOMO: -6.65318 LUMO: 1.93473 factor:1 | 1 (-2.97853) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.14924 HOMO: -6.18515 LUMO: 2.01364 factor:1 | 1 (-3.40316) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.55453 HOMO: -7.05591 LUMO: 2.13337 factor:1 | 1 (-2.80846) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51989 HOMO: -6.90897 LUMO: 2.29664 factor:1 | 1 (-2.77382) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52411 HOMO: -7.11034 LUMO: 2.17147 factor:1 | 1 (-2.77804) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.64381 HOMO: -6.82734 LUMO: 2.26671 factor:1 | 1 (-2.89774) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.25375 HOMO: -6.34842 LUMO: 2.34562 factor:1 | 1 (-0.50768) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.48465 HOMO: -6.62053 LUMO: 2.22861 factor:1 | 1 (-2.73858) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.18760 HOMO: -6.80557 LUMO: 2.07079 factor:1 | 1 (-0.44153) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56611 HOMO: -6.60692 LUMO: 2.46263 factor:1 | 1 (-0.82004) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.83500 HOMO: -7.02054 LUMO: 2.08711 factor:1 | 1 (-3.08893) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39677 HOMO: -6.78652 LUMO: 2.02453 factor:1 | 1 (-1.65070) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.46118 HOMO: -6.51168 LUMO: 2.06534 factor:1 | 1 (-1.71511) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52774 HOMO: -6.50080 LUMO: 2.01636 factor:1 | 1 (-1.78167) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.41896 HOMO: -6.54434 LUMO: 1.84493 factor:1 | 1 (-2.67289) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92935 HOMO: -6.47087 LUMO: 1.76330 factor:1 | 1 (-2.18328) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.73973 HOMO: -6.78924 LUMO: 2.39460 factor:1 | 1 (-2.99366) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.96720 HOMO: -6.59876 LUMO: 1.84493 factor:1 | 1 (-2.22113) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89210 HOMO: -6.41644 LUMO: 2.05174 factor:1 | 1 (-2.14603) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.49072 HOMO: -6.52257 LUMO: 2.11160 factor:1 | -1 (0.25535) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.73587 HOMO: -6.90897 LUMO: 2.34018 factor:1 | -1 (0.01020) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.13966 HOMO: -6.97428 LUMO: 1.86126 factor:1 | 1 (-0.39359) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.83845 HOMO: -7.13483 LUMO: 2.14698 factor:1 | 1 (-0.09238) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.23406 HOMO: -7.16748 LUMO: 2.31841 factor:1 | -1 (0.51201) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.33719 HOMO: -6.87087 LUMO: 2.38916 factor:1 | -1 (0.40888) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.08085 HOMO: -6.93074 LUMO: 2.42181 factor:1 | 1 (-0.33478) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.51418 HOMO: -6.90081 LUMO: 2.00276 factor:1 | -1 (0.23190) | 1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.68732 HOMO: -6.99333 LUMO: 2.03541 factor:1 | -1 (0.05875) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.80019 HOMO: -6.89264 LUMO: 1.57554 factor:1 | 1 (-1.05411) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.79480 HOMO: -6.48175 LUMO: 1.85854 factor:1 | 1 (-1.04873) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.50682 HOMO: -6.69400 LUMO: 1.62452 factor:1 | 1 (-0.76075) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.63036 HOMO: -6.50896 LUMO: 1.88303 factor:1 | 1 (-0.88429) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.30325 HOMO: -6.60420 LUMO: 2.05990 factor:1 | 1 (-0.55718) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46551 HOMO: -7.14299 LUMO: 2.07351 factor:1 | 1 (-0.71944) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.65169 HOMO: -7.06408 LUMO: 1.81228 factor:1 | 1 (-0.90562) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49520 HOMO: -6.67495 LUMO: 1.79595 factor:1 | 1 (-0.74913) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44894 HOMO: -6.45182 LUMO: 2.15786 factor:1 | 1 (-0.70287) | -1 | -1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86116 HOMO: -6.93346 LUMO: 2.45719 factor:1 | 1 (-2.11509) | 1 | 1 |
| G: -5245.38038 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68135 HOMO: -6.50080 LUMO: 2.08167 factor:1 | 1 (-1.93527) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79316 HOMO: -6.83550 LUMO: -0.67484 factor:1 | 1 (-2.04709) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.79264 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-2.04657) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.62422 HOMO: -6.79740 LUMO: 1.91296 factor:1 | 1 (-2.87815) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98473 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-2.23865) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92470 HOMO: -6.62597 LUMO: -0.44082 factor:1 | 1 (-2.17863) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91749 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-2.17141) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92399 HOMO: -6.51168 LUMO: -0.23130 factor:1 | 1 (-2.17792) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95879 HOMO: -7.14027 LUMO: 0.49797 factor:1 | 1 (-2.21272) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89675 HOMO: -7.55660 LUMO: 0.24762 factor:1 | 1 (-2.15068) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65740 HOMO: -6.88992 LUMO: -0.64763 factor:1 | 1 (-1.91133) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68181 HOMO: -6.72665 LUMO: -0.45987 factor:1 | 1 (-1.93574) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41476 HOMO: -6.72121 LUMO: -0.58232 factor:1 | 1 (-1.66868) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67269 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-1.92662) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40507 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-1.65900) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.32676 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-0.58069) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.46143 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-0.71536) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.69227 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-0.94619) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.64380 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-0.89773) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38821 HOMO: -6.79740 LUMO: -0.55511 factor:1 | 1 (-0.64213) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.73246 HOMO: -6.79740 LUMO: -0.67756 factor:1 | 1 (-0.98639) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40652 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-0.66045) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44119 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-0.69511) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.12404 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-0.37797) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.20420 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-0.45813) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58236 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-0.83629) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.32018 HOMO: -6.59332 LUMO: -0.27211 factor:1 | 1 (-0.57411) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19280 HOMO: -6.57427 LUMO: -0.16871 factor:1 | 1 (-0.44673) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44728 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-0.70121) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.22905 HOMO: -6.72121 LUMO: 2.00004 factor:1 | 1 (-0.48297) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.60075 HOMO: -6.61509 LUMO: 1.55921 factor:1 | 1 (-0.85468) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71553 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-0.96946) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39803 HOMO: -6.66135 LUMO: 2.02181 factor:1 | 1 (-0.65196) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.95069 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-1.20462) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71831 HOMO: -6.66679 LUMO: 1.98371 factor:1 | 1 (-0.97224) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.70802 HOMO: -6.67495 LUMO: 2.04085 factor:1 | 1 (-0.96195) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52502 HOMO: -6.89809 LUMO: 1.95106 factor:1 | 1 (-1.77894) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.05393 HOMO: -6.50352 LUMO: 1.88847 factor:1 | 1 (-1.30786) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29198 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-1.54591) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.35825 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-0.61217) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54764 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-0.80157) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.57542 HOMO: -6.65591 LUMO: 2.20684 factor:1 | 1 (-0.82935) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33855 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-0.59247) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33387 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-0.58779) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40339 HOMO: -6.53617 LUMO: 1.75241 factor:1 | 1 (-0.65732) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85060 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-2.10453) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67375 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-1.92768) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.34843 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-2.60236) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.19340 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-3.44733) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.09155 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-3.34548) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68613 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-2.94005) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45472 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-2.70865) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.68056 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-1.93448) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.41675 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-0.67068) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.66565 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-0.91958) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55343 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-0.80736) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51188 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-0.76581) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.30140 HOMO: -6.90897 LUMO: 1.91296 factor:1 | 1 (-0.55533) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.31093 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-0.56485) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31388 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-1.56781) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.35824 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-1.61217) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64192 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-1.89584) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38945 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-1.64338) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.16256 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-1.41649) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50521 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-1.75913) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.15598 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-1.40990) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.25565 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-1.50958) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.92832 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-1.18225) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12985 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-1.38378) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65563 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-1.90956) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52289 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-1.77682) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.25305 HOMO: -6.75387 LUMO: 1.72248 factor:1 | 1 (-3.50698) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.40816 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-2.66209) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.52313 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-2.77706) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.61222 HOMO: -6.80557 LUMO: 2.02725 factor:1 | 1 (-2.86615) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.65282 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-2.90675) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66831 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-1.92224) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49136 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-1.74528) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.62105 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-1.87497) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.91606 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-3.16999) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64842 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-1.90235) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.73724 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-1.99117) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93860 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-2.19253) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.67051 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-2.92443) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52930 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-0.78323) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49199 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-0.74592) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12832 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-2.38225) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29734 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-1.55127) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.49944 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-1.75337) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33505 HOMO: -6.64230 LUMO: 2.16058 factor:1 | 1 (-1.58898) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.60245 HOMO: -6.58788 LUMO: 2.10616 factor:1 | -1 (0.14362) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.63763 HOMO: -7.01782 LUMO: 2.13609 factor:1 | -1 (0.10844) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.26488 HOMO: -6.31304 LUMO: 2.31841 factor:1 | 1 (-0.51881) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19326 HOMO: -6.94979 LUMO: 2.07895 factor:1 | 1 (-0.44719) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49553 HOMO: -6.88992 LUMO: 2.28031 factor:1 | 1 (-0.74946) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.21286 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-0.46678) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.02485 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-0.27878) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38029 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-0.63422) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.55430 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-1.80822) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52053 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-1.77445) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.38185 HOMO: -6.31304 LUMO: 2.18507 factor:1 | -1 (0.36422) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.28046 HOMO: -6.18243 LUMO: 2.01636 factor:1 | -1 (0.46561) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.09451 HOMO: -6.99877 LUMO: 2.14970 factor:1 | 1 (-0.34844) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.98357 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-0.23750) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57823 HOMO: -6.36202 LUMO: 2.17419 factor:1 | 1 (-2.83216) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83052 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-2.08445) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70439 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-1.95832) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29228 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-1.54621) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.40363 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-1.65755) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37212 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-1.62604) | 1 | 1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36608 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-0.62001) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17686 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-0.43078) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.24932 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-0.50325) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.02235 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-0.27628) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.45045 HOMO: -6.44094 LUMO: 1.74425 factor:1 | 1 (-2.70438) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52464 HOMO: -6.51985 LUMO: 1.84221 factor:1 | 1 (-1.77856) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.77449 HOMO: -6.63414 LUMO: -0.24762 factor:1 | 1 (-2.02842) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71759 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-1.97152) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53770 HOMO: -7.19741 LUMO: 0.58232 factor:1 | 1 (-1.79162) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48107 HOMO: -6.77019 LUMO: -0.56872 factor:1 | 1 (-1.73500) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.31151 HOMO: -7.46136 LUMO: 0.28844 factor:1 | 1 (-2.56544) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.13841 HOMO: -6.60420 LUMO: -0.54151 factor:1 | 1 (-0.39233) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.05775 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-0.31168) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19242 HOMO: -6.81645 LUMO: -0.57144 factor:1 | 1 (-0.44635) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.70437 HOMO: -7.48041 LUMO: 0.28572 factor:1 | 1 (-1.95829) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.36648 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-1.62041) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41565 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-1.66958) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.93264 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-2.18657) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.72330 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-2.97722) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81561 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-2.06953) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91757 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-2.17150) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.12019 HOMO: -6.50896 LUMO: -0.25034 factor:1 | 1 (-1.37412) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.97796 HOMO: -7.17564 LUMO: -0.68573 factor:1 | 1 (-1.23189) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.97521 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-1.22914) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.17543 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-1.42936) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.44970 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-0.70363) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.57273 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-0.82665) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.52296 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-0.77689) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.86919 HOMO: -6.62325 LUMO: 2.02725 factor:1 | 1 (-1.12312) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36023 HOMO: -6.63414 LUMO: 1.91296 factor:1 | 1 (-0.61416) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.22135 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-0.47527) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29299 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-0.54692) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19090 HOMO: -6.61237 LUMO: 2.11432 factor:1 | 1 (-0.44482) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92021 HOMO: -6.62053 LUMO: 2.09256 factor:1 | 1 (-2.17414) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85425 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-2.10817) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.80384 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-3.05777) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89196 HOMO: -6.85183 LUMO: 2.12793 factor:1 | 1 (-2.14589) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.02081 HOMO: -6.81101 LUMO: 1.83949 factor:1 | 1 (-2.27474) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71422 HOMO: -6.98788 LUMO: 2.16058 factor:1 | 1 (-1.96815) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65737 HOMO: -6.62869 LUMO: 2.00820 factor:1 | 1 (-1.91130) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72731 HOMO: -6.34025 LUMO: 2.25855 factor:1 | 1 (-1.98123) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.67506 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-1.92899) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.27445 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-2.52837) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.16239 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-2.41632) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.20410 HOMO: -6.83278 LUMO: 1.53744 factor:1 | 1 (-2.45803) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12092 HOMO: -6.41917 LUMO: 1.82316 factor:1 | 1 (-2.37485) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08282 HOMO: -6.56339 LUMO: 1.63813 factor:1 | 1 (-2.33675) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.13869 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-2.39262) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.01719 HOMO: -6.63141 LUMO: 1.92112 factor:1 | 1 (-2.27112) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.63187 HOMO: -6.83822 LUMO: 1.88847 factor:1 | 1 (-2.88579) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.68006 HOMO: -6.84638 LUMO: 1.90480 factor:1 | 1 (-2.93399) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.58212 HOMO: -6.82462 LUMO: 1.70888 factor:1 | 1 (-2.83605) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.57167 HOMO: -6.82734 LUMO: 2.12521 factor:1 | 1 (-2.82560) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.07343 HOMO: -6.94435 LUMO: 1.87214 factor:1 | 1 (-2.32736) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72973 HOMO: -6.98516 LUMO: 2.51433 factor:1 | 1 (-1.98366) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26436 HOMO: -6.74026 LUMO: 2.15514 factor:1 | 1 (-1.51829) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26912 HOMO: -6.93618 LUMO: 2.54426 factor:1 | 1 (-1.52305) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89074 HOMO: -6.28583 LUMO: 2.53610 factor:1 | 1 (-2.14467) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09679 HOMO: -6.56883 LUMO: 1.94834 factor:1 | 1 (-1.35072) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28841 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-1.54234) | 1 | 1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11559 HOMO: -6.19059 LUMO: 1.99732 factor:1 | 1 (-1.36952) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33579 HOMO: -6.78108 LUMO: 2.03813 factor:1 | 1 (-1.58972) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.68085 HOMO: -6.82189 LUMO: 1.77418 factor:1 | -1 (0.06523) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.52735 HOMO: -6.45454 LUMO: 1.78779 factor:1 | -1 (0.21873) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.16415 HOMO: -6.84366 LUMO: 1.77690 factor:1 | 1 (-0.41808) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.15710 HOMO: -6.74026 LUMO: 1.67622 factor:1 | 1 (-0.41103) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.83930 HOMO: -6.76475 LUMO: 2.40277 factor:1 | 1 (-3.09323) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.05743 HOMO: -6.65863 LUMO: 1.86670 factor:1 | 1 (-2.31136) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89509 HOMO: -6.50080 LUMO: 1.93201 factor:1 | 1 (-2.14902) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72660 HOMO: -6.34842 LUMO: 1.70888 factor:1 | 1 (-1.98053) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86510 HOMO: -6.60692 LUMO: 2.20140 factor:1 | 1 (-2.11903) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82679 HOMO: -6.74026 LUMO: 2.14970 factor:1 | 1 (-2.08072) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74956 HOMO: -6.63686 LUMO: 2.17419 factor:1 | 1 (-2.00349) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40415 HOMO: -6.81917 LUMO: 2.10072 factor:1 | 1 (-0.65808) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.29827 HOMO: -6.92802 LUMO: 2.04358 factor:1 | 1 (-0.55220) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43759 HOMO: -6.56067 LUMO: -0.47620 factor:1 | 1 (-0.69152) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.56628 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-0.82021) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.76010 HOMO: -6.78380 LUMO: -0.64763 factor:1 | 1 (-2.01402) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75868 HOMO: -6.51985 LUMO: -0.24490 factor:1 | 1 (-2.01261) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74595 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-1.99987) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48820 HOMO: -7.10489 LUMO: -0.62586 factor:1 | 1 (-1.74213) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81708 HOMO: -7.18108 LUMO: 0.48980 factor:1 | 1 (-2.07100) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71623 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-1.97016) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.94892 HOMO: -6.70761 LUMO: -0.54423 factor:1 | 1 (-2.20284) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.91920 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-2.17313) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.61722 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-0.87115) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.54456 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-0.79849) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58214 HOMO: -6.77836 LUMO: -0.54423 factor:1 | 1 (-0.83607) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62217 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-0.87610) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41448 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-1.66841) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.41726 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-1.67119) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.51585 HOMO: -6.66951 LUMO: -0.40817 factor:1 | 1 (-1.76977) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32069 HOMO: -6.60420 LUMO: -0.19320 factor:1 | 1 (-1.57461) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.26466 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-1.51859) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.34251 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-1.59644) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.27241 HOMO: -7.27088 LUMO: 0.53334 factor:1 | 1 (-1.52634) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.95887 HOMO: -7.20013 LUMO: 0.59049 factor:1 | 1 (-2.21280) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.19109 HOMO: -6.60148 LUMO: -0.20953 factor:1 | 1 (-3.44502) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51241 HOMO: -6.69400 LUMO: -0.51974 factor:1 | 1 (-2.76634) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.42226 HOMO: -7.40422 LUMO: -0.98777 factor:1 | 1 (-2.67619) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.51518 HOMO: -6.88176 LUMO: -0.71022 factor:1 | 1 (-2.76911) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.83574 HOMO: -6.86271 LUMO: -0.59321 factor:1 | 1 (-2.08967) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58338 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-1.83731) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.63250 HOMO: -6.71033 LUMO: 1.57010 factor:1 | 1 (-1.88643) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.58602 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-1.83995) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.58021 HOMO: -6.67495 LUMO: 2.03813 factor:1 | 1 (-0.83414) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.39142 HOMO: -6.54434 LUMO: 1.83677 factor:1 | 1 (-0.64535) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40646 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-0.66039) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88807 HOMO: -6.76747 LUMO: 1.87759 factor:1 | 1 (-2.14200) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.44474 HOMO: -6.58243 LUMO: 1.61364 factor:1 | 1 (-1.69867) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.31407 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-1.56800) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42390 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-1.67783) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45119 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-1.70512) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.42956 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-1.68349) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.56845 HOMO: -6.83278 LUMO: 1.91296 factor:1 | 1 (-1.82237) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53081 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-1.78474) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81852 HOMO: -6.50080 LUMO: 1.73337 factor:1 | 1 (-2.07245) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.69650 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-1.95043) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.00337 HOMO: -6.63686 LUMO: 2.20140 factor:1 | 1 (-2.25729) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82755 HOMO: -6.57427 LUMO: 1.87214 factor:1 | 1 (-2.08148) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64837 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-1.90229) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75833 HOMO: -6.63958 LUMO: 2.04902 factor:1 | 1 (-2.01225) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.53645 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-1.79037) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.85961 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-2.11354) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.98323 HOMO: -6.72938 LUMO: 2.28304 factor:1 | 1 (-2.23716) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.61149 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-2.86541) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.99381 HOMO: -6.95523 LUMO: 2.33474 factor:1 | 1 (-2.24774) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11513.05536 HOMO: -6.59876 LUMO: 2.30480 factor:1 | 1 (-3.30929) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.23755 HOMO: -6.87360 LUMO: 1.75786 factor:1 | -1 (1.50852) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.63100 HOMO: -7.06408 LUMO: 1.99187 factor:1 | -1 (1.11507) | 1 | 1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.52681 HOMO: -6.95795 LUMO: 1.88847 factor:1 | -1 (1.21926) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.45174 HOMO: -6.85455 LUMO: 1.63813 factor:1 | -1 (1.29434) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.14346 HOMO: -7.09129 LUMO: 2.31569 factor:1 | -1 (1.60261) | 1 | 1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.44602 HOMO: -6.91441 LUMO: 1.68983 factor:1 | -1 (1.30005) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.69676 HOMO: -6.89809 LUMO: 2.23678 factor:1 | -1 (0.04931) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.93405 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-0.18798) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.47202 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-0.72595) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11507.77678 HOMO: -7.07224 LUMO: 2.13337 factor:1 | -1 (1.96929) | 1 | 1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11507.88952 HOMO: -6.94979 LUMO: 2.28031 factor:1 | -1 (1.85655) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.04544 HOMO: -6.60965 LUMO: 2.20412 factor:1 | -1 (1.70063) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.39217 HOMO: -6.87360 LUMO: 2.40277 factor:1 | -1 (1.35390) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.55963 HOMO: -6.92802 LUMO: 1.89663 factor:1 | -1 (1.18644) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.40364 HOMO: -6.88448 LUMO: 2.02725 factor:1 | -1 (0.34243) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.00222 HOMO: -6.69128 LUMO: 1.55105 factor:1 | -1 (0.74385) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.48048 HOMO: -6.54978 LUMO: 1.93201 factor:1 | 1 (-0.73441) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.45506 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-0.70899) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.71455 HOMO: -6.55794 LUMO: 1.89663 factor:1 | 1 (-0.96848) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.57991 HOMO: -6.07630 LUMO: 1.94289 factor:1 | 1 (-0.83384) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.43553 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-0.68945) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.69335 HOMO: -6.63958 LUMO: -0.61770 factor:1 | 1 (-0.94728) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.83564 HOMO: -6.81101 LUMO: -0.57960 factor:1 | 1 (-1.08957) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.69273 HOMO: -6.74298 LUMO: -0.57960 factor:1 | 1 (-0.94666) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.02068 HOMO: -6.63686 LUMO: -0.42994 factor:1 | 1 (-1.27461) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.40138 HOMO: -6.60965 LUMO: -0.41089 factor:1 | 1 (-0.65530) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.67754 HOMO: -6.60692 LUMO: -0.80274 factor:1 | 1 (-0.93147) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.62821 HOMO: -6.58788 LUMO: -0.78097 factor:1 | 1 (-0.88214) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.00305 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-1.25698) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.51540 HOMO: -6.63141 LUMO: -0.40545 factor:1 | -1 (0.23067) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.64471 HOMO: -6.62053 LUMO: -0.83811 factor:1 | -1 (0.10136) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.72977 HOMO: -6.59604 LUMO: -0.35375 factor:1 | -1 (0.01630) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.72172 HOMO: -6.34297 LUMO: -0.39729 factor:1 | -1 (0.02435) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.33195 HOMO: -6.67223 LUMO: 1.97827 factor:1 | -1 (1.41412) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.86366 HOMO: -6.40012 LUMO: 1.89935 factor:1 | -1 (0.88241) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.79615 HOMO: -6.74842 LUMO: 1.97283 factor:1 | -1 (0.94992) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.96900 HOMO: -6.76747 LUMO: 2.17147 factor:1 | -1 (0.77708) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11508.84597 HOMO: -6.72121 LUMO: 1.55649 factor:1 | -1 (0.90010) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34445 HOMO: -6.97700 LUMO: 2.04085 factor:1 | 1 (-0.59838) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51523 HOMO: -7.06680 LUMO: 2.04085 factor:1 | 1 (-0.76916) | 1 | 1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.36652 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-0.62045) | 1 | 1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.34418 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.59811) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33969 HOMO: -6.72665 LUMO: 2.20140 factor:1 | 1 (-0.59362) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.42508 HOMO: -6.77291 LUMO: 2.34562 factor:1 | 1 (-0.67901) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.11845 HOMO: -6.73754 LUMO: 2.00276 factor:1 | 1 (-1.37238) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.22751 HOMO: -7.04231 LUMO: 1.92112 factor:1 | 1 (-2.48143) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.09323 HOMO: -6.83822 LUMO: 1.72248 factor:1 | 1 (-1.34715) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.29538 HOMO: -6.57971 LUMO: 2.16603 factor:1 | 1 (-1.54931) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.32681 HOMO: -6.80013 LUMO: 1.88575 factor:1 | 1 (-1.58074) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.21462 HOMO: -6.93618 LUMO: 2.18235 factor:1 | 1 (-1.46854) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33094 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-1.58487) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.50015 HOMO: -7.06952 LUMO: 2.18507 factor:1 | 1 (-1.75407) | 1 | 1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.38869 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-1.64262) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.92723 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-2.18116) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.89623 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-2.15016) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.81222 HOMO: -7.17292 LUMO: 1.90752 factor:1 | 1 (-3.06615) | 1 | 1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.74701 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-2.00093) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.82263 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-2.07656) | 1 | 1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.75512 HOMO: -6.85727 LUMO: 2.13609 factor:1 | 1 (-2.00904) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.86113 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-2.11506) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.01113 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-1.26506) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.33571 HOMO: -6.67223 LUMO: 2.07351 factor:1 | 1 (-1.58963) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.08296 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-2.33689) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11512.12903 HOMO: -6.90897 LUMO: 2.28848 factor:1 | 1 (-2.38296) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11509.95911 HOMO: -7.04231 LUMO: 1.70071 factor:1 | 1 (-0.21304) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.32908 HOMO: -6.69944 LUMO: 1.94834 factor:1 | 1 (-0.58300) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.45549 HOMO: -6.56067 LUMO: 2.20956 factor:1 | 1 (-1.70942) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39666 HOMO: -6.65046 LUMO: 2.06807 factor:1 | 1 (-1.65059) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.30030 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-1.55423) | 1 | 1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39590 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-1.64983) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48496 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-1.73889) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.39495 HOMO: -6.85183 LUMO: 2.16058 factor:1 | 1 (-1.64887) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.81933 HOMO: -6.54706 LUMO: 1.92384 factor:1 | 1 (-2.07326) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.06569 HOMO: -6.84366 LUMO: 2.48984 factor:1 | 1 (-1.31962) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.28724 HOMO: -6.77291 LUMO: 2.46263 factor:1 | 1 (-1.54117) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.72110 HOMO: -7.01782 LUMO: 2.31025 factor:1 | 1 (-1.97503) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.66701 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-1.92093) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.65936 HOMO: -6.64230 LUMO: 1.97283 factor:1 | 1 (-1.91329) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.51044 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-0.76437) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.32089 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-0.57481) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.38655 HOMO: -7.17020 LUMO: 2.06807 factor:1 | 1 (-0.64047) | 1 | 1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.18499 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-0.43892) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.48551 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-1.73943) | 1 | 1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.64842 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-1.90235) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.37263 HOMO: -6.92802 LUMO: 1.99187 factor:1 | 1 (-1.62656) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.17120 HOMO: -6.69672 LUMO: 2.36739 factor:1 | 1 (-0.42512) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.08001 HOMO: -7.13755 LUMO: 2.00276 factor:1 | 1 (-0.33394) | 1 | 1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.33019 HOMO: -6.92530 LUMO: 2.25582 factor:1 | 1 (-0.58412) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.19596 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-0.44989) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.87319 HOMO: -6.87904 LUMO: 1.60003 factor:1 | 1 (-2.12711) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.52036 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-1.77429) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.88989 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-2.14382) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11511.71109 HOMO: -6.74298 LUMO: 1.47486 factor:1 | 1 (-1.96502) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.55455 HOMO: -6.77019 LUMO: 1.90480 factor:1 | 1 (-0.80848) | -1 | -1 |
| G: -5245.38038 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11510.49409 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-0.74801) | -1 | -1 |