乙二醇作为反应物的反应表19-6

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

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| 反应物A | 反应物B | 产物C | Gibbs自由能判据(ΔG) | 前线轨道理论判据 | 是否同时满足 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90601 HOMO: -6.91169 LUMO: -0.53879 factor:1 | 1 (-0.03840) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.38239 HOMO: -7.29809 LUMO: 2.83543 factor:1 | 1 (-1.51478) | 1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.12173 HOMO: -6.86543 LUMO: -0.70205 factor:1 | 1 (-2.25411) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18598 HOMO: -7.47769 LUMO: 0.31293 factor:1 | 1 (-1.31836) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87199 HOMO: -6.63141 LUMO: -0.55511 factor:1 | 1 (-1.00437) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68464 HOMO: -6.68856 LUMO: -0.30205 factor:1 | 1 (-0.81702) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91944 HOMO: -7.22190 LUMO: 0.53334 factor:1 | -1 (0.94818) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10888 HOMO: -6.66407 LUMO: -0.27756 factor:1 | -1 (0.75874) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05801 HOMO: -7.15659 LUMO: -0.70205 factor:1 | 1 (-1.19039) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84554 HOMO: -6.69400 LUMO: 1.67622 factor:1 | 1 (-0.97792) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.99451 HOMO: -6.60420 LUMO: 2.16058 factor:1 | -1 (0.87310) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.11854 HOMO: -6.87087 LUMO: 1.88031 factor:1 | -1 (0.74908) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.96888 HOMO: -6.60965 LUMO: -0.19864 factor:1 | -1 (0.89874) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80683 HOMO: -7.29265 LUMO: 0.52246 factor:1 | -1 (0.06079) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96079 HOMO: -6.86543 LUMO: -0.59593 factor:1 | 1 (-0.09317) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85243 HOMO: -7.44504 LUMO: -1.01226 factor:1 | -1 (0.01518) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.40030 HOMO: -6.92530 LUMO: -0.75103 factor:1 | 1 (-1.53268) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.88844 HOMO: -7.10489 LUMO: 2.20412 factor:1 | 1 (-2.02083) | 1 | 1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.04258 HOMO: -6.58788 LUMO: 1.73881 factor:1 | 1 (-1.17496) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.63416 HOMO: -6.64502 LUMO: 1.70343 factor:1 | 1 (-0.76654) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79069 HOMO: -6.73754 LUMO: 1.60819 factor:1 | -1 (0.07693) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05736 HOMO: -6.80829 LUMO: 2.45991 factor:1 | 1 (-0.18974) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71506 HOMO: -6.91713 LUMO: 2.43814 factor:1 | 1 (-0.84744) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.66134 HOMO: -6.60692 LUMO: 1.93745 factor:1 | 1 (-1.79372) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74877 HOMO: -6.26134 LUMO: 1.46125 factor:1 | 1 (-0.88116) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.00562 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-1.13801) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.54778 HOMO: -6.97700 LUMO: -0.73471 factor:1 | 1 (-1.68017) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83193 HOMO: -6.92258 LUMO: -0.70205 factor:1 | 1 (-0.96432) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79152 HOMO: -6.83550 LUMO: -0.56872 factor:1 | 1 (-0.92391) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97218 HOMO: -6.72121 LUMO: 1.89663 factor:1 | 1 (-1.10456) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19140 HOMO: -6.73482 LUMO: 1.89935 factor:1 | 1 (-0.32379) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35192 HOMO: -6.61781 LUMO: 1.86670 factor:1 | 1 (-0.48431) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27606 HOMO: -7.01782 LUMO: 2.26399 factor:1 | 1 (-0.40844) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96805 HOMO: -7.23551 LUMO: 2.09800 factor:1 | 1 (-0.10044) | 1 | 1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.63879 HOMO: -7.13483 LUMO: 2.17963 factor:1 | 1 (-0.77117) | 1 | 1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73667 HOMO: -6.22869 LUMO: 2.01092 factor:1 | 1 (-0.86905) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.50237 HOMO: -6.80285 LUMO: 2.14970 factor:1 | 1 (-1.63475) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52520 HOMO: -7.21102 LUMO: 2.33746 factor:1 | 1 (-1.65758) | 1 | 1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68986 HOMO: -6.39740 LUMO: 2.59597 factor:1 | 1 (-0.82225) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24946 HOMO: -7.07768 LUMO: 2.48168 factor:1 | 1 (-1.38185) | 1 | 1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.43285 HOMO: -7.11306 LUMO: 0.90614 factor:1 | 1 (-0.56523) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22722 HOMO: -6.61781 LUMO: -2.46263 factor:1 | -1 (0.64039) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32290 HOMO: -6.96611 LUMO: 0.90614 factor:1 | -1 (0.54472) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.74735 HOMO: -6.86271 LUMO: -1.14832 factor:1 | -1 (1.12027) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.95089 HOMO: -6.72665 LUMO: 0.96873 factor:1 | -1 (0.91672) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.15899 HOMO: -7.14571 LUMO: 1.05036 factor:1 | -1 (1.70863) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.46275 HOMO: -7.14299 LUMO: 0.98777 factor:1 | -1 (1.40487) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.58041 HOMO: -6.99333 LUMO: 1.05852 factor:1 | -1 (1.28721) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12519.95817 HOMO: -6.78924 LUMO: -1.49935 factor:1 | -1 (1.90945) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.76474 HOMO: -7.13755 LUMO: 0.94151 factor:1 | -1 (1.10288) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.69033 HOMO: -6.72938 LUMO: -0.35375 factor:1 | -1 (0.17728) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52715 HOMO: -6.99061 LUMO: 0.82450 factor:1 | -1 (0.34047) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22268 HOMO: -6.75114 LUMO: -0.68028 factor:1 | -1 (0.64494) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.25642 HOMO: -6.40556 LUMO: -0.42722 factor:1 | -1 (0.61119) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36867 HOMO: -7.18653 LUMO: 0.42178 factor:1 | -1 (0.49895) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.06727 HOMO: -6.63958 LUMO: -0.71294 factor:1 | -1 (0.80034) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.41313 HOMO: -6.63958 LUMO: -0.71022 factor:1 | -1 (0.45448) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91459 HOMO: -6.69672 LUMO: -0.72654 factor:1 | -1 (0.95302) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12621 HOMO: -6.56883 LUMO: -0.80274 factor:1 | -1 (0.74140) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24186 HOMO: -6.68584 LUMO: -0.56872 factor:1 | -1 (0.62575) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.04869 HOMO: -6.59060 LUMO: -0.35647 factor:1 | -1 (0.81893) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.78368 HOMO: -6.72121 LUMO: -0.71838 factor:1 | -1 (1.08394) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34143 HOMO: -6.57971 LUMO: -0.61498 factor:1 | -1 (0.52619) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.65409 HOMO: -7.07496 LUMO: 0.50613 factor:1 | -1 (0.21353) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.75327 HOMO: -7.14027 LUMO: 0.43266 factor:1 | -1 (0.11434) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39299 HOMO: -6.43277 LUMO: -0.44082 factor:1 | -1 (0.47462) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78699 HOMO: -6.79468 LUMO: 0.07619 factor:1 | -1 (0.08063) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91513 HOMO: -6.81917 LUMO: -2.57148 factor:1 | 1 (-0.04751) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48183 HOMO: -6.71849 LUMO: 1.30615 factor:1 | 1 (-0.61422) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57239 HOMO: -6.85455 LUMO: -0.63675 factor:1 | 1 (-0.70477) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75835 HOMO: -6.73210 LUMO: -1.03131 factor:1 | 1 (-0.89074) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58996 HOMO: -6.83550 LUMO: -0.58777 factor:1 | 1 (-1.72234) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.53565 HOMO: -6.53073 LUMO: -0.74287 factor:1 | 1 (-1.66803) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69680 HOMO: -7.18381 LUMO: -0.92791 factor:1 | 1 (-0.82919) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41922 HOMO: -6.49264 LUMO: -0.44627 factor:1 | 1 (-0.55160) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53179 HOMO: -7.32803 LUMO: 0.41361 factor:1 | 1 (-0.66418) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75865 HOMO: -6.53073 LUMO: -0.52790 factor:1 | 1 (-0.89104) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73710 HOMO: -6.54978 LUMO: -0.53062 factor:1 | 1 (-0.86949) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61745 HOMO: -6.56611 LUMO: -0.37824 factor:1 | 1 (-0.74984) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30879 HOMO: -6.57155 LUMO: -0.64219 factor:1 | 1 (-0.44118) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53174 HOMO: -7.08040 LUMO: 0.45715 factor:1 | 1 (-0.66412) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.37905 HOMO: -6.66679 LUMO: -0.75376 factor:1 | 1 (-0.51144) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42733 HOMO: -6.83550 LUMO: -0.99322 factor:1 | 1 (-0.55971) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31301 HOMO: -6.53345 LUMO: -0.29660 factor:1 | 1 (-0.44540) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30907 HOMO: -6.65046 LUMO: 2.40549 factor:1 | 1 (-0.44145) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40817 HOMO: -6.98788 LUMO: 2.01092 factor:1 | 1 (-0.54055) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54755 HOMO: -6.61781 LUMO: 1.92384 factor:1 | 1 (-0.67993) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.20281 HOMO: -6.61237 LUMO: 2.06807 factor:1 | 1 (-0.33519) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34948 HOMO: -6.59060 LUMO: 1.95106 factor:1 | -1 (0.51813) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12768 HOMO: -6.48175 LUMO: 1.72248 factor:1 | -1 (0.73993) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12474 HOMO: -6.84911 LUMO: 2.03541 factor:1 | -1 (0.74287) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83395 HOMO: -6.50624 LUMO: 2.17147 factor:1 | 1 (-0.96633) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58820 HOMO: -6.68312 LUMO: 2.08439 factor:1 | 1 (-0.72058) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28184 HOMO: -6.96067 LUMO: 1.98099 factor:1 | -1 (0.58578) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26004 HOMO: -6.93618 LUMO: 1.85854 factor:1 | -1 (0.60758) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68183 HOMO: -6.71305 LUMO: -0.61226 factor:1 | 1 (-0.81422) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30994 HOMO: -7.06408 LUMO: 0.80001 factor:1 | 1 (-0.44232) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76053 HOMO: -6.52257 LUMO: 0.99049 factor:1 | 1 (-0.89291) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42861 HOMO: -6.84638 LUMO: 1.10750 factor:1 | 1 (-0.56099) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18885 HOMO: -6.85455 LUMO: 0.84900 factor:1 | 1 (-0.32123) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.50170 HOMO: -6.60148 LUMO: -0.78369 factor:1 | -1 (0.36591) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36208 HOMO: -6.86543 LUMO: -0.93063 factor:1 | -1 (0.50553) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.47719 HOMO: -6.70489 LUMO: -0.72382 factor:1 | -1 (0.39043) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.14836 HOMO: -6.59060 LUMO: 0.31293 factor:1 | -1 (0.71925) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.27950 HOMO: -6.52257 LUMO: -0.48708 factor:1 | -1 (0.58812) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20603 HOMO: -6.54706 LUMO: -0.48164 factor:1 | -1 (0.66159) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.41621 HOMO: -7.32803 LUMO: 0.08436 factor:1 | -1 (0.45141) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.47961 HOMO: -6.77291 LUMO: -0.66940 factor:1 | -1 (0.38801) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.72666 HOMO: -6.68312 LUMO: -0.53062 factor:1 | -1 (0.14095) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01263 HOMO: -7.07768 LUMO: 0.45987 factor:1 | 1 (-0.14501) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25663 HOMO: -6.50352 LUMO: -0.63675 factor:1 | 1 (-0.38901) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33117 HOMO: -6.48992 LUMO: -0.60681 factor:1 | -1 (0.53645) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39381 HOMO: -6.65318 LUMO: -0.72382 factor:1 | -1 (0.47380) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.25571 HOMO: -6.54706 LUMO: 0.24218 factor:1 | -1 (0.61190) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.52382 HOMO: -6.63958 LUMO: 0.57416 factor:1 | 1 (-0.65620) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25768 HOMO: -6.37563 LUMO: -0.48164 factor:1 | 1 (-1.39007) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.11313 HOMO: -6.64774 LUMO: -0.71838 factor:1 | 1 (-2.24551) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.87350 HOMO: -7.17020 LUMO: 0.45987 factor:1 | 1 (-2.00589) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.45047 HOMO: -6.86543 LUMO: -1.05036 factor:1 | 1 (-2.58285) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.17819 HOMO: -6.77019 LUMO: -1.03131 factor:1 | 1 (-2.31057) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.99620 HOMO: -6.80285 LUMO: 1.05852 factor:1 | 1 (-2.12858) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30568 HOMO: -6.76475 LUMO: 1.01771 factor:1 | 1 (-1.43807) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.13141 HOMO: -6.92530 LUMO: 1.37417 factor:1 | 1 (-2.26380) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.64781 HOMO: -6.98244 LUMO: 1.25989 factor:1 | 1 (-1.78020) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39929 HOMO: -6.74842 LUMO: 0.89798 factor:1 | 1 (-1.53167) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36211 HOMO: -6.77019 LUMO: -1.17009 factor:1 | -1 (0.50551) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34856 HOMO: -6.78652 LUMO: 1.35785 factor:1 | -1 (0.51906) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33479 HOMO: -6.82734 LUMO: -0.68301 factor:1 | -1 (0.53283) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99083 HOMO: -6.48175 LUMO: -2.19052 factor:1 | 1 (-0.12321) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26240 HOMO: -6.65863 LUMO: -0.77008 factor:1 | 1 (-0.39478) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24847 HOMO: -6.44094 LUMO: -2.20956 factor:1 | 1 (-0.38085) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85934 HOMO: -6.59876 LUMO: -0.57688 factor:1 | -1 (0.00827) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36980 HOMO: -6.78380 LUMO: -0.77008 factor:1 | 1 (-0.50219) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06710 HOMO: -7.30354 LUMO: 0.25034 factor:1 | 1 (-0.19949) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91749 HOMO: -6.59332 LUMO: -0.53334 factor:1 | 1 (-0.04988) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22931 HOMO: -6.64230 LUMO: -0.55783 factor:1 | 1 (-0.36169) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85964 HOMO: -7.26544 LUMO: 0.20409 factor:1 | -1 (0.00797) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.96638 HOMO: -6.61237 LUMO: -0.65307 factor:1 | 1 (-2.09876) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06084 HOMO: -6.72393 LUMO: -0.65307 factor:1 | 1 (-1.19322) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24315 HOMO: -6.29671 LUMO: -0.39729 factor:1 | 1 (-1.37554) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.99555 HOMO: -6.75387 LUMO: -0.53334 factor:1 | 1 (-2.12793) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.99911 HOMO: -6.53073 LUMO: -0.31293 factor:1 | 1 (-2.13150) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12503 HOMO: -6.42189 LUMO: -0.59049 factor:1 | 1 (-1.25741) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.64798 HOMO: -6.41100 LUMO: -0.29933 factor:1 | 1 (-1.78036) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72741 HOMO: -6.57427 LUMO: -0.53879 factor:1 | 1 (-0.85980) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18712 HOMO: -7.43143 LUMO: 0.33470 factor:1 | 1 (-1.31951) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.38773 HOMO: -6.56067 LUMO: -0.50885 factor:1 | 1 (-1.52011) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44825 HOMO: -6.65863 LUMO: -0.76464 factor:1 | 1 (-0.58064) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33481 HOMO: -6.32665 LUMO: -0.41906 factor:1 | 1 (-0.46719) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30591 HOMO: -6.57699 LUMO: 1.63813 factor:1 | 1 (-0.43829) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01121 HOMO: -6.53073 LUMO: 1.71704 factor:1 | 1 (-0.14359) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.52251 HOMO: -6.86271 LUMO: 2.07351 factor:1 | 1 (-0.65490) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10285 HOMO: -6.63686 LUMO: 1.78235 factor:1 | 1 (-1.23523) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32762 HOMO: -6.60965 LUMO: 1.94289 factor:1 | 1 (-0.46001) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10093 HOMO: -6.55250 LUMO: 1.89119 factor:1 | 1 (-0.23331) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33230 HOMO: -6.50624 LUMO: 1.85582 factor:1 | 1 (-0.46469) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12519.99125 HOMO: -6.06814 LUMO: 1.94561 factor:1 | -1 (1.87636) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12519.98821 HOMO: -6.58788 LUMO: 2.01908 factor:1 | -1 (1.87941) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.57839 HOMO: -6.74026 LUMO: 0.31293 factor:1 | -1 (1.28922) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.86689 HOMO: -6.54434 LUMO: -0.42994 factor:1 | -1 (1.00073) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.54065 HOMO: -6.94707 LUMO: 0.42994 factor:1 | 1 (-1.67304) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35647 HOMO: -6.98516 LUMO: 0.41361 factor:1 | 1 (-0.48885) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57089 HOMO: -6.31304 LUMO: -0.54967 factor:1 | 1 (-0.70328) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16808 HOMO: -6.48447 LUMO: -0.40817 factor:1 | 1 (-0.30047) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00014 HOMO: -6.49264 LUMO: 0.29116 factor:1 | 1 (-0.13252) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19393 HOMO: -6.48719 LUMO: -0.11973 factor:1 | 1 (-0.32632) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.87835 HOMO: -7.16204 LUMO: 0.44082 factor:1 | -1 (0.98927) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.04390 HOMO: -6.74842 LUMO: -0.37552 factor:1 | -1 (0.82372) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.00278 HOMO: -6.44638 LUMO: -0.45171 factor:1 | -1 (0.86483) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29219 HOMO: -7.07496 LUMO: 0.50341 factor:1 | 1 (-1.42457) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53242 HOMO: -6.79468 LUMO: 0.11429 factor:1 | 1 (-0.66480) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03509 HOMO: -6.63958 LUMO: -0.67484 factor:1 | 1 (-1.16748) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22090 HOMO: -7.08584 LUMO: 0.46259 factor:1 | 1 (-0.35329) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56942 HOMO: -6.80285 LUMO: -0.73199 factor:1 | 1 (-0.70181) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32022 HOMO: -6.44366 LUMO: -0.45443 factor:1 | 1 (-0.45261) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33835 HOMO: -6.75931 LUMO: 0.25851 factor:1 | 1 (-0.47073) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32847 HOMO: -6.64502 LUMO: 1.79323 factor:1 | 1 (-0.46085) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46436 HOMO: -6.51168 LUMO: 1.60275 factor:1 | 1 (-0.59675) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13369 HOMO: -6.56067 LUMO: 1.63268 factor:1 | 1 (-0.26607) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11336 HOMO: -6.56883 LUMO: 1.70615 factor:1 | 1 (-0.24575) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26400 HOMO: -6.77836 LUMO: 1.77962 factor:1 | 1 (-0.39639) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01551 HOMO: -6.38923 LUMO: 1.85854 factor:1 | 1 (-0.14789) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14294 HOMO: -6.35658 LUMO: 2.16875 factor:1 | 1 (-0.27532) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33297 HOMO: -6.83006 LUMO: 2.31025 factor:1 | -1 (0.53465) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.31362 HOMO: -6.87087 LUMO: 1.79051 factor:1 | -1 (0.55400) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29944 HOMO: -6.56339 LUMO: 2.37828 factor:1 | -1 (0.56817) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28584 HOMO: -6.30488 LUMO: 2.51705 factor:1 | -1 (0.58178) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.25239 HOMO: -6.69400 LUMO: 1.95650 factor:1 | -1 (0.61522) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10540 HOMO: -6.51168 LUMO: 2.03541 factor:1 | -1 (0.76222) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61168 HOMO: -6.30760 LUMO: 1.65173 factor:1 | 1 (-0.74407) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60034 HOMO: -6.55250 LUMO: 1.90752 factor:1 | 1 (-0.73272) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24716 HOMO: -6.41372 LUMO: 1.76058 factor:1 | 1 (-0.37954) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29144 HOMO: -6.23957 LUMO: 2.06534 factor:1 | -1 (0.57617) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.90425 HOMO: -6.58243 LUMO: 2.11705 factor:1 | -1 (0.96336) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09919 HOMO: -6.37835 LUMO: 2.09256 factor:1 | -1 (0.76842) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.17898 HOMO: -6.50624 LUMO: 2.55787 factor:1 | -1 (0.68864) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69441 HOMO: -6.45454 LUMO: 1.87214 factor:1 | 1 (-0.82679) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27225 HOMO: -6.53617 LUMO: 1.95650 factor:1 | 1 (-0.40463) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71808 HOMO: -6.51985 LUMO: 1.71432 factor:1 | 1 (-0.85046) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84035 HOMO: -6.75114 LUMO: 1.84493 factor:1 | -1 (0.02727) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07880 HOMO: -6.06270 LUMO: 1.65717 factor:1 | 1 (-0.21119) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57528 HOMO: -5.89671 LUMO: 1.71704 factor:1 | 1 (-0.70766) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77556 HOMO: -6.18787 LUMO: 1.91840 factor:1 | -1 (0.09206) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15622 HOMO: -6.01644 LUMO: 1.85582 factor:1 | 1 (-0.28860) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96484 HOMO: -6.05998 LUMO: 2.33474 factor:1 | 1 (-0.09723) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80110 HOMO: -6.05725 LUMO: 2.03541 factor:1 | 1 (-0.93349) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57598 HOMO: -6.80829 LUMO: 1.90480 factor:1 | 1 (-0.70837) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26346 HOMO: -6.76475 LUMO: 2.20956 factor:1 | 1 (-0.39584) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07312 HOMO: -6.29944 LUMO: 1.77962 factor:1 | 1 (-0.20550) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.70291 HOMO: -6.47359 LUMO: -0.25579 factor:1 | -1 (1.16470) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24352 HOMO: -6.57699 LUMO: -0.47348 factor:1 | -1 (0.62409) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.90101 HOMO: -7.20830 LUMO: 0.49797 factor:1 | -1 (0.96660) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18964 HOMO: -7.49402 LUMO: 0.29933 factor:1 | 1 (-0.32202) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10776 HOMO: -6.66679 LUMO: -0.58777 factor:1 | 1 (-0.24014) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25282 HOMO: -6.67767 LUMO: -0.56328 factor:1 | 1 (-0.38520) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14299 HOMO: -7.42871 LUMO: 0.35647 factor:1 | 1 (-0.27538) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95924 HOMO: -6.56067 LUMO: -0.54423 factor:1 | 1 (-0.09162) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32969 HOMO: -6.56339 LUMO: -0.50341 factor:1 | 1 (-0.46208) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71090 HOMO: -6.56067 LUMO: -0.48436 factor:1 | 1 (-0.84328) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39152 HOMO: -6.73210 LUMO: 1.75241 factor:1 | 1 (-0.52390) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86285 HOMO: -6.48175 LUMO: 1.91296 factor:1 | -1 (0.00476) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17864 HOMO: -6.67767 LUMO: 1.70343 factor:1 | 1 (-0.31103) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67092 HOMO: -6.37835 LUMO: 1.96466 factor:1 | 1 (-0.80331) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.85631 HOMO: -6.40828 LUMO: 2.10072 factor:1 | 1 (-0.98870) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91014 HOMO: -6.06542 LUMO: 1.92112 factor:1 | 1 (-1.04252) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.82777 HOMO: -6.90353 LUMO: 1.83133 factor:1 | 1 (-0.96015) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48360 HOMO: -6.37019 LUMO: 1.92929 factor:1 | 1 (-0.61598) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.82774 HOMO: -6.61509 LUMO: 2.11160 factor:1 | 1 (-0.96013) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80586 HOMO: -6.82734 LUMO: 1.77146 factor:1 | 1 (-0.93825) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10880 HOMO: -6.01100 LUMO: 1.89935 factor:1 | -1 (0.75882) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21830 HOMO: -6.49536 LUMO: 1.75241 factor:1 | -1 (0.64932) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.83448 HOMO: -6.34297 LUMO: 1.86398 factor:1 | -1 (1.03313) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38478 HOMO: -6.53073 LUMO: 1.84493 factor:1 | -1 (0.48284) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91688 HOMO: -6.53345 LUMO: 2.41093 factor:1 | -1 (0.95074) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.75040 HOMO: -7.01237 LUMO: 2.06262 factor:1 | -1 (1.11722) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.96765 HOMO: -6.17154 LUMO: 1.89119 factor:1 | -1 (0.89996) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78579 HOMO: -6.08719 LUMO: 1.74425 factor:1 | -1 (0.08182) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16363 HOMO: -6.69672 LUMO: 1.95106 factor:1 | -1 (0.70399) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15362 HOMO: -6.58243 LUMO: 2.24766 factor:1 | -1 (0.71400) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39340 HOMO: -6.74570 LUMO: 2.02181 factor:1 | -1 (0.47421) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84914 HOMO: -6.53890 LUMO: 1.92929 factor:1 | -1 (0.01848) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.69807 HOMO: -6.03276 LUMO: 1.67078 factor:1 | -1 (1.16955) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79423 HOMO: -6.67767 LUMO: 2.03541 factor:1 | -1 (0.07339) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77575 HOMO: -5.98378 LUMO: 1.84221 factor:1 | -1 (0.09187) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86163 HOMO: -6.07086 LUMO: 2.01908 factor:1 | -1 (0.00599) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.57018 HOMO: -6.29944 LUMO: 1.90208 factor:1 | -1 (1.29744) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.78409 HOMO: -6.75114 LUMO: 1.85854 factor:1 | -1 (1.08353) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.64659 HOMO: -6.56611 LUMO: 2.49801 factor:1 | -1 (1.22103) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.78956 HOMO: -6.39740 LUMO: 1.92929 factor:1 | -1 (1.07806) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.57924 HOMO: -6.85999 LUMO: -1.07757 factor:1 | -1 (1.28838) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48007 HOMO: -6.98244 LUMO: 1.07213 factor:1 | -1 (0.38754) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.71986 HOMO: -7.04231 LUMO: 0.64219 factor:1 | -1 (0.14776) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.68832 HOMO: -6.96339 LUMO: 0.75648 factor:1 | -1 (0.17930) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80963 HOMO: -6.83822 LUMO: -0.97417 factor:1 | -1 (0.05799) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52282 HOMO: -6.44910 LUMO: -2.15242 factor:1 | -1 (0.34480) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24246 HOMO: -6.84094 LUMO: -1.37690 factor:1 | -1 (0.62515) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13242 HOMO: -6.74026 LUMO: -2.54699 factor:1 | -1 (0.73520) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39071 HOMO: -6.96611 LUMO: 1.24900 factor:1 | -1 (0.47691) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.47515 HOMO: -7.21102 LUMO: 0.82995 factor:1 | -1 (0.39247) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13343 HOMO: -6.88448 LUMO: 0.81634 factor:1 | -1 (0.73419) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34649 HOMO: -7.04231 LUMO: 1.10750 factor:1 | -1 (0.52113) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91880 HOMO: -6.83550 LUMO: -0.98777 factor:1 | 1 (-0.05118) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17004 HOMO: -6.82189 LUMO: 0.93879 factor:1 | 1 (-0.30243) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.70247 HOMO: -6.81101 LUMO: 0.70750 factor:1 | -1 (0.16515) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93322 HOMO: -7.06680 LUMO: 0.74015 factor:1 | 1 (-0.06561) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94160 HOMO: -6.68856 LUMO: 0.86260 factor:1 | 1 (-0.07399) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.76896 HOMO: -6.83822 LUMO: -0.63403 factor:1 | -1 (1.09866) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.98725 HOMO: -6.84911 LUMO: 1.26533 factor:1 | -1 (0.88037) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36067 HOMO: -7.01237 LUMO: 0.73743 factor:1 | -1 (0.50695) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43354 HOMO: -7.00965 LUMO: 1.40139 factor:1 | -1 (0.43408) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43852 HOMO: -6.73210 LUMO: -2.49256 factor:1 | -1 (0.42910) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38987 HOMO: -7.08040 LUMO: 0.84627 factor:1 | -1 (0.47775) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57327 HOMO: -7.00965 LUMO: 0.82995 factor:1 | -1 (0.29435) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22633 HOMO: -6.88448 LUMO: 0.82723 factor:1 | -1 (0.64129) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44930 HOMO: -7.20013 LUMO: 0.88437 factor:1 | -1 (0.41832) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13625 HOMO: -6.60420 LUMO: -0.53334 factor:1 | 1 (-0.26863) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87992 HOMO: -6.78652 LUMO: -0.79729 factor:1 | 1 (-0.01230) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27954 HOMO: -6.48992 LUMO: -0.64491 factor:1 | 1 (-0.41193) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04751 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-0.17989) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.37865 HOMO: -6.65046 LUMO: -0.78097 factor:1 | 1 (-0.51103) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.40431 HOMO: -7.24095 LUMO: 0.37280 factor:1 | -1 (0.46330) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13532 HOMO: -6.81101 LUMO: -0.74831 factor:1 | 1 (-0.26771) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55790 HOMO: -6.69400 LUMO: -0.77280 factor:1 | -1 (0.30972) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82321 HOMO: -6.08447 LUMO: -0.68573 factor:1 | -1 (0.04441) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30137 HOMO: -6.66679 LUMO: -0.47076 factor:1 | 1 (-0.43375) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57545 HOMO: -6.97428 LUMO: -1.10750 factor:1 | -1 (0.29217) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80040 HOMO: -6.69128 LUMO: -0.54151 factor:1 | -1 (0.06721) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.60731 HOMO: -6.53617 LUMO: -0.35375 factor:1 | -1 (0.26030) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83167 HOMO: -6.75659 LUMO: -0.41361 factor:1 | -1 (0.03595) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06465 HOMO: -6.69400 LUMO: -0.67484 factor:1 | 1 (-0.19704) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02860 HOMO: -6.89264 LUMO: -0.90886 factor:1 | 1 (-0.16098) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22449 HOMO: -6.56339 LUMO: -0.52518 factor:1 | 1 (-0.35688) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27791 HOMO: -6.45726 LUMO: -0.65852 factor:1 | 1 (-0.41029) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.64649 HOMO: -6.80557 LUMO: -0.56600 factor:1 | 1 (-0.77887) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78986 HOMO: -7.19469 LUMO: -0.91702 factor:1 | 1 (-0.92225) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75827 HOMO: -6.41100 LUMO: 0.79185 factor:1 | 1 (-0.89066) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50164 HOMO: -6.39195 LUMO: 0.26123 factor:1 | 1 (-0.63403) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42621 HOMO: -6.78924 LUMO: 0.35919 factor:1 | 1 (-0.55860) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12842 HOMO: -6.50624 LUMO: 0.71838 factor:1 | -1 (0.73920) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13451 HOMO: -6.68584 LUMO: -0.66124 factor:1 | -1 (0.73310) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12891 HOMO: -6.45182 LUMO: -0.48980 factor:1 | -1 (0.73871) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09672 HOMO: -7.18925 LUMO: -1.01498 factor:1 | -1 (0.77090) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09557 HOMO: -7.18925 LUMO: -0.63130 factor:1 | -1 (0.77204) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.82395 HOMO: -6.66679 LUMO: -0.57960 factor:1 | -1 (1.04367) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29133 HOMO: -6.44910 LUMO: -0.30205 factor:1 | -1 (0.57628) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.41155 HOMO: -7.23279 LUMO: 0.46804 factor:1 | -1 (0.45606) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48810 HOMO: -6.92802 LUMO: -0.72927 factor:1 | -1 (0.37952) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38206 HOMO: -6.83278 LUMO: -0.59321 factor:1 | -1 (0.48556) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.95013 HOMO: -7.44776 LUMO: 0.27211 factor:1 | -1 (0.91749) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37615 HOMO: -6.80829 LUMO: -0.59865 factor:1 | -1 (0.49146) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30322 HOMO: -6.63686 LUMO: -0.75103 factor:1 | -1 (0.56439) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.08004 HOMO: -6.73210 LUMO: -0.55511 factor:1 | -1 (0.78758) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.99448 HOMO: -6.50624 LUMO: 1.58642 factor:1 | -1 (0.87313) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.64174 HOMO: -6.79196 LUMO: 0.96328 factor:1 | -1 (1.22587) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38494 HOMO: -6.82734 LUMO: 1.23540 factor:1 | -1 (0.48268) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.07364 HOMO: -6.90081 LUMO: 1.25444 factor:1 | -1 (0.79397) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24091 HOMO: -7.00965 LUMO: -1.05036 factor:1 | -1 (0.62671) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43403 HOMO: -7.01237 LUMO: -1.48302 factor:1 | -1 (0.43359) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.66144 HOMO: -6.91713 LUMO: 0.93607 factor:1 | -1 (0.20618) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16610 HOMO: -7.02598 LUMO: 0.92247 factor:1 | 1 (-0.29848) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10242 HOMO: -6.98516 LUMO: 1.52384 factor:1 | 1 (-0.23481) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11293 HOMO: -6.75387 LUMO: 1.04764 factor:1 | 1 (-0.24531) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.76734 HOMO: -7.09401 LUMO: 1.19458 factor:1 | -1 (0.10027) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90438 HOMO: -6.88992 LUMO: -1.56193 factor:1 | 1 (-0.03676) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83140 HOMO: -7.00149 LUMO: 0.99866 factor:1 | -1 (0.03622) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77567 HOMO: -7.13755 LUMO: 1.05308 factor:1 | -1 (0.09195) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.54625 HOMO: -6.85183 LUMO: -1.42860 factor:1 | -1 (0.32137) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.64500 HOMO: -6.63141 LUMO: -0.88981 factor:1 | -1 (0.22262) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.81880 HOMO: -6.92258 LUMO: -0.82178 factor:1 | -1 (0.04882) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93611 HOMO: -6.55794 LUMO: -0.80818 factor:1 | 1 (-0.06849) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87099 HOMO: -6.95251 LUMO: -0.97145 factor:1 | 1 (-0.00337) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28226 HOMO: -7.37701 LUMO: 0.14150 factor:1 | 1 (-0.41465) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59685 HOMO: -6.74842 LUMO: -0.68028 factor:1 | 1 (-0.72924) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.49753 HOMO: -6.65046 LUMO: -0.52518 factor:1 | 1 (-0.62992) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28264 HOMO: -6.91441 LUMO: -1.13199 factor:1 | 1 (-0.41503) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59933 HOMO: -7.00965 LUMO: -1.00682 factor:1 | 1 (-0.73171) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39603 HOMO: -6.55794 LUMO: -0.54967 factor:1 | 1 (-0.52842) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08694 HOMO: -6.71577 LUMO: -0.53879 factor:1 | 1 (-0.21932) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.57189 HOMO: -6.88992 LUMO: -0.55511 factor:1 | 1 (-1.70428) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69528 HOMO: -6.74026 LUMO: -0.60681 factor:1 | 1 (-0.82766) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44295 HOMO: -6.76747 LUMO: -0.50885 factor:1 | 1 (-0.57533) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30410 HOMO: -6.87904 LUMO: -0.92519 factor:1 | 1 (-1.43649) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60521 HOMO: -6.53073 LUMO: -0.53062 factor:1 | 1 (-0.73759) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58257 HOMO: -6.97700 LUMO: -0.98505 factor:1 | 1 (-0.71495) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38539 HOMO: -6.96884 LUMO: -0.79185 factor:1 | 1 (-0.51778) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56417 HOMO: -6.60420 LUMO: -0.31021 factor:1 | 1 (-0.69656) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58934 HOMO: -6.68584 LUMO: -0.63947 factor:1 | 1 (-0.72173) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69413 HOMO: -6.41917 LUMO: -0.35103 factor:1 | 1 (-0.82652) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28523 HOMO: -6.73482 LUMO: -0.70477 factor:1 | 1 (-0.41761) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39241 HOMO: -6.71305 LUMO: -0.85716 factor:1 | 1 (-0.52480) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30256 HOMO: -6.70761 LUMO: -0.63403 factor:1 | 1 (-0.43495) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46583 HOMO: -6.37563 LUMO: -0.38640 factor:1 | 1 (-0.59822) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41018 HOMO: -6.27495 LUMO: -0.54967 factor:1 | 1 (-0.54257) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17611 HOMO: -6.98516 LUMO: 0.38096 factor:1 | 1 (-0.30850) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14789 HOMO: -6.47087 LUMO: -0.40001 factor:1 | 1 (-0.28028) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.81581 HOMO: -6.59876 LUMO: 0.20681 factor:1 | -1 (1.05180) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.72553 HOMO: -6.89809 LUMO: 0.14966 factor:1 | -1 (1.14209) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12842 HOMO: -6.76203 LUMO: 2.11432 factor:1 | -1 (0.73920) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.01106 HOMO: -6.58516 LUMO: 1.75786 factor:1 | -1 (0.85656) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.64194 HOMO: -6.37835 LUMO: 1.84493 factor:1 | 1 (-0.77433) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31394 HOMO: -6.83550 LUMO: 1.74425 factor:1 | 1 (-0.44632) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.72142 HOMO: -6.65318 LUMO: 1.79051 factor:1 | -1 (1.14620) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.03982 HOMO: -6.68584 LUMO: 2.11160 factor:1 | -1 (0.82780) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59707 HOMO: -6.36202 LUMO: 1.85037 factor:1 | 1 (-0.72946) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60611 HOMO: -6.68312 LUMO: 2.23133 factor:1 | 1 (-0.73849) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31415 HOMO: -6.66679 LUMO: 2.14154 factor:1 | 1 (-0.44654) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80106 HOMO: -6.50896 LUMO: 1.92657 factor:1 | -1 (0.06656) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04800 HOMO: -6.63686 LUMO: 2.22317 factor:1 | 1 (-0.18038) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38154 HOMO: -6.58788 LUMO: 2.17419 factor:1 | -1 (0.48608) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22290 HOMO: -6.72665 LUMO: 2.12249 factor:1 | -1 (0.64472) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26619 HOMO: -6.28311 LUMO: 1.91024 factor:1 | -1 (0.60143) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.31169 HOMO: -6.56067 LUMO: 2.27487 factor:1 | -1 (0.55593) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.97179 HOMO: -6.83006 LUMO: 2.28031 factor:1 | -1 (0.89583) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.08839 HOMO: -6.45182 LUMO: 1.62724 factor:1 | -1 (0.77923) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.23130 HOMO: -6.78380 LUMO: 1.83677 factor:1 | -1 (0.63631) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26377 HOMO: -6.23413 LUMO: 1.80956 factor:1 | -1 (0.60385) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30820 HOMO: -6.74298 LUMO: 2.16875 factor:1 | 1 (-0.44058) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40931 HOMO: -6.81645 LUMO: 2.50073 factor:1 | 1 (-0.54170) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19854 HOMO: -6.71033 LUMO: 1.96466 factor:1 | -1 (0.66907) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.35161 HOMO: -6.83550 LUMO: 2.04358 factor:1 | -1 (0.51601) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06871 HOMO: -6.60965 LUMO: 2.38100 factor:1 | 1 (-0.20109) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04452 HOMO: -6.73210 LUMO: 2.26127 factor:1 | 1 (-0.17690) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07567 HOMO: -6.76203 LUMO: 2.13609 factor:1 | 1 (-0.20806) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23423 HOMO: -6.71033 LUMO: 2.05990 factor:1 | 1 (-0.36662) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.89606 HOMO: -6.50896 LUMO: 2.32385 factor:1 | 1 (-2.02845) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11518 HOMO: -6.53345 LUMO: 1.74425 factor:1 | 1 (-1.24756) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.88746 HOMO: -6.25862 LUMO: 1.63540 factor:1 | 1 (-2.01985) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58035 HOMO: -5.90759 LUMO: 1.78779 factor:1 | 1 (-1.71274) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.77128 HOMO: -6.09807 LUMO: 1.99732 factor:1 | 1 (-0.90366) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02312 HOMO: -5.92392 LUMO: 1.99732 factor:1 | 1 (-1.15550) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.35826 HOMO: -6.45182 LUMO: 1.72248 factor:1 | 1 (-1.49064) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30741 HOMO: -6.53073 LUMO: 1.82588 factor:1 | 1 (-0.43979) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08291 HOMO: -6.40828 LUMO: 2.05174 factor:1 | 1 (-0.21530) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85461 HOMO: -6.60420 LUMO: -0.82450 factor:1 | -1 (0.01301) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55727 HOMO: -6.76747 LUMO: -0.57144 factor:1 | -1 (0.31035) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02626 HOMO: -6.67767 LUMO: -0.59321 factor:1 | 1 (-0.15864) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.85138 HOMO: -6.65863 LUMO: -0.57416 factor:1 | -1 (1.01624) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.88790 HOMO: -6.49808 LUMO: -0.54695 factor:1 | -1 (0.97972) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19171 HOMO: -6.50080 LUMO: -0.61498 factor:1 | -1 (0.67590) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.07617 HOMO: -6.74842 LUMO: -0.51974 factor:1 | -1 (0.79144) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.86537 HOMO: -6.13345 LUMO: 0.67756 factor:1 | -1 (1.00225) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21824 HOMO: -6.48719 LUMO: 0.52790 factor:1 | -1 (0.64937) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.58871 HOMO: -6.35930 LUMO: 0.74015 factor:1 | -1 (1.27891) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.44783 HOMO: -6.41644 LUMO: 0.22313 factor:1 | -1 (1.41978) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.18450 HOMO: -6.85727 LUMO: -0.00272 factor:1 | -1 (0.68311) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34480 HOMO: -6.84638 LUMO: 0.24762 factor:1 | -1 (0.52281) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15830 HOMO: -6.66951 LUMO: 0.39184 factor:1 | -1 (0.70932) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22714 HOMO: -6.62597 LUMO: -0.65035 factor:1 | -1 (0.64047) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.06975 HOMO: -7.13755 LUMO: 0.45715 factor:1 | -1 (0.79787) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.14504 HOMO: -7.12666 LUMO: 0.45171 factor:1 | -1 (0.72257) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.00194 HOMO: -6.46270 LUMO: -0.46259 factor:1 | -1 (0.86568) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16994 HOMO: -6.36202 LUMO: -0.29660 factor:1 | -1 (0.69767) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.84000 HOMO: -6.28583 LUMO: 0.40545 factor:1 | -1 (1.02761) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22940 HOMO: -6.70761 LUMO: 0.41906 factor:1 | -1 (0.63822) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87594 HOMO: -6.76203 LUMO: -0.60954 factor:1 | 1 (-0.00833) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52913 HOMO: -6.85999 LUMO: -0.75103 factor:1 | -1 (0.33848) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46840 HOMO: -7.19741 LUMO: -1.00954 factor:1 | -1 (0.39922) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.70008 HOMO: -6.58243 LUMO: -0.33470 factor:1 | -1 (0.16754) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.67206 HOMO: -7.22190 LUMO: 0.49253 factor:1 | -1 (1.19556) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.81837 HOMO: -7.22462 LUMO: 0.51974 factor:1 | -1 (1.04924) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.58835 HOMO: -7.08584 LUMO: -0.68301 factor:1 | -1 (1.27926) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.71219 HOMO: -6.68584 LUMO: -0.29660 factor:1 | -1 (1.15542) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.34840 HOMO: -6.33753 LUMO: -0.48436 factor:1 | -1 (1.51921) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.79644 HOMO: -7.15932 LUMO: 0.55511 factor:1 | -1 (1.07118) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.41063 HOMO: -6.57427 LUMO: 2.01908 factor:1 | -1 (0.45699) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45985 HOMO: -6.75659 LUMO: 2.22045 factor:1 | -1 (0.40776) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.22299 HOMO: -6.73482 LUMO: 2.20956 factor:1 | -1 (1.64463) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.26223 HOMO: -6.74026 LUMO: 1.76602 factor:1 | -1 (1.60539) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55009 HOMO: -6.95523 LUMO: 1.94834 factor:1 | -1 (0.31753) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48652 HOMO: -6.33209 LUMO: 1.87486 factor:1 | -1 (0.38110) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.23831 HOMO: -6.71033 LUMO: 2.12521 factor:1 | -1 (1.62931) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.17224 HOMO: -6.50080 LUMO: 2.04902 factor:1 | -1 (1.69538) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12519.76121 HOMO: -6.76475 LUMO: 1.94017 factor:1 | -1 (2.10641) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12519.74943 HOMO: -6.53073 LUMO: 2.08983 factor:1 | -1 (2.11819) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12519.98584 HOMO: -6.69944 LUMO: 2.20684 factor:1 | -1 (1.88178) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36091 HOMO: -6.34570 LUMO: 1.80684 factor:1 | -1 (0.50670) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46875 HOMO: -6.78380 LUMO: 1.95922 factor:1 | -1 (0.39886) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57346 HOMO: -6.93618 LUMO: 1.76058 factor:1 | -1 (0.29416) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58103 HOMO: -6.93346 LUMO: 1.79595 factor:1 | -1 (0.28659) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39675 HOMO: -6.29671 LUMO: 1.75241 factor:1 | -1 (0.47087) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22173 HOMO: -6.77019 LUMO: 1.74697 factor:1 | -1 (0.64589) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26886 HOMO: -6.87360 LUMO: 1.91024 factor:1 | -1 (0.59876) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32771 HOMO: -6.32665 LUMO: 1.87759 factor:1 | -1 (0.53990) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19694 HOMO: -6.99877 LUMO: 1.99187 factor:1 | -1 (0.67068) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.04793 HOMO: -6.72665 LUMO: 2.12521 factor:1 | -1 (0.81969) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.87606 HOMO: -6.67767 LUMO: 2.43814 factor:1 | -1 (0.99156) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.52231 HOMO: -6.99605 LUMO: 1.79051 factor:1 | -1 (1.34530) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.96232 HOMO: -6.25046 LUMO: 1.77146 factor:1 | -1 (0.90530) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92920 HOMO: -6.30488 LUMO: 1.90480 factor:1 | 1 (-0.06158) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24115 HOMO: -6.38379 LUMO: 1.68438 factor:1 | 1 (-0.37353) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44921 HOMO: -6.78924 LUMO: 2.01364 factor:1 | -1 (0.41840) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.72715 HOMO: -6.15249 LUMO: 1.98643 factor:1 | -1 (0.14047) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.59663 HOMO: -6.19331 LUMO: 2.14154 factor:1 | -1 (1.27099) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.65255 HOMO: -6.05998 LUMO: 2.12521 factor:1 | -1 (1.21507) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.55924 HOMO: -6.67223 LUMO: 1.91840 factor:1 | -1 (1.30838) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.36843 HOMO: -6.79196 LUMO: 2.18507 factor:1 | -1 (1.49918) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.93723 HOMO: -6.93346 LUMO: 1.78235 factor:1 | -1 (0.93038) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.82890 HOMO: -6.16882 LUMO: 1.80956 factor:1 | -1 (1.03871) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28263 HOMO: -6.72665 LUMO: 2.07895 factor:1 | -1 (0.58499) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37245 HOMO: -6.73210 LUMO: 1.97827 factor:1 | -1 (0.49517) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98441 HOMO: -6.84638 LUMO: 1.87214 factor:1 | 1 (-0.11679) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24923 HOMO: -6.83006 LUMO: 2.36195 factor:1 | 1 (-0.38161) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19440 HOMO: -6.97700 LUMO: 1.91024 factor:1 | 1 (-0.32678) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41198 HOMO: -6.20420 LUMO: 1.81772 factor:1 | 1 (-0.54436) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.81047 HOMO: -7.09129 LUMO: 2.10344 factor:1 | -1 (0.05714) | 1 | 1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58247 HOMO: -6.77564 LUMO: 2.14970 factor:1 | -1 (0.28515) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53185 HOMO: -6.81645 LUMO: 1.85854 factor:1 | -1 (0.33576) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46959 HOMO: -6.50896 LUMO: 2.04358 factor:1 | -1 (0.39802) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82887 HOMO: -6.89264 LUMO: 1.66262 factor:1 | -1 (0.03875) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74184 HOMO: -6.75931 LUMO: 2.23950 factor:1 | -1 (0.12577) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45104 HOMO: -6.50080 LUMO: 1.67622 factor:1 | -1 (0.41658) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10738 HOMO: -6.30216 LUMO: 2.24222 factor:1 | -1 (0.76023) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78345 HOMO: -7.18108 LUMO: 2.10072 factor:1 | -1 (0.08416) | 1 | 1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.42434 HOMO: -6.54162 LUMO: 2.35378 factor:1 | -1 (0.44327) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27369 HOMO: -5.98650 LUMO: 1.48302 factor:1 | 1 (-0.40608) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45916 HOMO: -7.15115 LUMO: 2.14970 factor:1 | 1 (-0.59155) | 1 | 1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.45233 HOMO: -6.45454 LUMO: 2.15786 factor:1 | 1 (-1.58471) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61068 HOMO: -7.06952 LUMO: 2.14970 factor:1 | 1 (-0.74306) | 1 | 1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.54016 HOMO: -6.93618 LUMO: 1.86942 factor:1 | 1 (-1.67255) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47974 HOMO: -6.63141 LUMO: 1.92657 factor:1 | 1 (-0.61212) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37858 HOMO: -6.51441 LUMO: -0.44355 factor:1 | 1 (-1.51097) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39815 HOMO: -6.82734 LUMO: -1.03131 factor:1 | 1 (-1.53053) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12405 HOMO: -6.58788 LUMO: -0.82995 factor:1 | 1 (-1.25643) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19010 HOMO: -6.43277 LUMO: -0.40817 factor:1 | 1 (-0.32248) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30822 HOMO: -6.78924 LUMO: -0.72110 factor:1 | 1 (-0.44061) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88647 HOMO: -7.28177 LUMO: 0.36735 factor:1 | 1 (-0.01886) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44401 HOMO: -6.47903 LUMO: -0.46259 factor:1 | 1 (-0.57639) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.93195 HOMO: -6.67495 LUMO: -0.75376 factor:1 | 1 (-2.06434) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.89900 HOMO: -6.71033 LUMO: -0.71838 factor:1 | 1 (-2.03138) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.98254 HOMO: -6.79740 LUMO: -0.79185 factor:1 | 1 (-2.11492) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.44698 HOMO: -6.08719 LUMO: -0.63675 factor:1 | 1 (-2.57937) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15485 HOMO: -6.84094 LUMO: 0.42994 factor:1 | 1 (-1.28723) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.74330 HOMO: -6.59604 LUMO: 0.25851 factor:1 | 1 (-1.87568) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.03043 HOMO: -6.82462 LUMO: 0.08708 factor:1 | 1 (-2.16282) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25072 HOMO: -6.54706 LUMO: 0.44082 factor:1 | 1 (-1.38310) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72581 HOMO: -6.99333 LUMO: 0.32109 factor:1 | 1 (-0.85819) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67762 HOMO: -6.29944 LUMO: -0.57144 factor:1 | 1 (-0.81000) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39013 HOMO: -6.57699 LUMO: -0.46531 factor:1 | 1 (-0.52251) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40376 HOMO: -6.24773 LUMO: -0.53879 factor:1 | 1 (-0.53615) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.29108 HOMO: -6.96067 LUMO: -0.67212 factor:1 | 1 (-0.42346) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.43516 HOMO: -7.24095 LUMO: -0.09252 factor:1 | 1 (-0.56755) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.04883 HOMO: -6.33481 LUMO: -0.46531 factor:1 | 1 (-2.18121) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25368 HOMO: -6.43549 LUMO: -0.33198 factor:1 | 1 (-1.38607) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.07400 HOMO: -6.53073 LUMO: 0.44899 factor:1 | 1 (-2.20638) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.18385 HOMO: -6.69128 LUMO: 0.47620 factor:1 | 1 (-2.31623) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33308 HOMO: -6.65318 LUMO: 0.52246 factor:1 | 1 (-1.46547) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.02298 HOMO: -6.71305 LUMO: 0.41089 factor:1 | 1 (-2.15536) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07460 HOMO: -6.70216 LUMO: 0.19864 factor:1 | 1 (-1.20699) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27254 HOMO: -6.41100 LUMO: 0.34558 factor:1 | 1 (-1.40492) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37452 HOMO: -7.01237 LUMO: 0.02993 factor:1 | -1 (0.49310) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16730 HOMO: -6.85999 LUMO: 0.18776 factor:1 | -1 (0.70031) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30456 HOMO: -6.62869 LUMO: 0.48708 factor:1 | -1 (0.56306) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19543 HOMO: -6.43821 LUMO: -0.45715 factor:1 | 1 (-0.32782) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98688 HOMO: -6.43277 LUMO: -0.72110 factor:1 | 1 (-0.11927) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25317 HOMO: -7.10761 LUMO: 0.43266 factor:1 | 1 (-0.38556) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11018 HOMO: -6.57699 LUMO: -0.61498 factor:1 | 1 (-0.24256) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85153 HOMO: -6.82189 LUMO: -0.75648 factor:1 | -1 (0.01608) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97635 HOMO: -6.55794 LUMO: -0.67212 factor:1 | 1 (-0.10874) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07845 HOMO: -6.69128 LUMO: 1.88575 factor:1 | 1 (-0.21083) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.22100 HOMO: -6.65591 LUMO: 1.70888 factor:1 | 1 (-1.35339) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.12845 HOMO: -6.58788 LUMO: 1.68438 factor:1 | 1 (-2.26083) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.18613 HOMO: -6.46270 LUMO: 1.72520 factor:1 | 1 (-2.31852) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.70961 HOMO: -6.57427 LUMO: 1.73881 factor:1 | 1 (-1.84199) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96208 HOMO: -6.45182 LUMO: 1.75241 factor:1 | 1 (-1.09447) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15469 HOMO: -6.51441 LUMO: 1.78779 factor:1 | 1 (-1.28707) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.34944 HOMO: -6.67495 LUMO: 2.11705 factor:1 | 1 (-1.48182) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57389 HOMO: -6.22597 LUMO: 1.96466 factor:1 | 1 (-0.70627) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28907 HOMO: -6.68040 LUMO: 2.30753 factor:1 | -1 (0.57854) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11597 HOMO: -6.65046 LUMO: 2.18235 factor:1 | 1 (-0.24836) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33824 HOMO: -6.38651 LUMO: 1.76874 factor:1 | 1 (-0.47062) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92623 HOMO: -6.41644 LUMO: 2.09256 factor:1 | 1 (-0.05861) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26936 HOMO: -6.14977 LUMO: 2.28031 factor:1 | 1 (-0.40175) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54926 HOMO: -6.70489 LUMO: 2.43814 factor:1 | 1 (-0.68165) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28270 HOMO: -6.78924 LUMO: 2.27215 factor:1 | 1 (-0.41508) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93959 HOMO: -6.86271 LUMO: 2.31025 factor:1 | 1 (-0.07197) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58608 HOMO: -6.51168 LUMO: 2.04630 factor:1 | 1 (-0.71846) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38948 HOMO: -6.72665 LUMO: 2.13337 factor:1 | 1 (-0.52186) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38616 HOMO: -6.45998 LUMO: 2.16058 factor:1 | 1 (-0.51854) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61239 HOMO: -6.83822 LUMO: 2.20684 factor:1 | 1 (-0.74478) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75329 HOMO: -6.68856 LUMO: 2.19324 factor:1 | 1 (-0.88568) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26011 HOMO: -6.71577 LUMO: 2.16058 factor:1 | 1 (-0.39250) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.51138 HOMO: -6.82462 LUMO: 1.90208 factor:1 | 1 (-0.64377) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.52638 HOMO: -6.61509 LUMO: 2.23950 factor:1 | 1 (-0.65876) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.43054 HOMO: -6.73754 LUMO: 1.84221 factor:1 | 1 (-0.56292) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28116 HOMO: -6.56611 LUMO: 1.94561 factor:1 | -1 (0.58646) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.93492 HOMO: -6.67767 LUMO: 1.51840 factor:1 | -1 (0.93270) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.27778 HOMO: -6.35658 LUMO: 2.16603 factor:1 | -1 (0.58983) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67617 HOMO: -6.35114 LUMO: 2.08983 factor:1 | 1 (-0.80856) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27347 HOMO: -6.35114 LUMO: 2.10616 factor:1 | 1 (-0.40586) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47742 HOMO: -6.71305 LUMO: 2.01636 factor:1 | 1 (-0.60981) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93477 HOMO: -6.24773 LUMO: 1.98915 factor:1 | 1 (-0.06716) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24109 HOMO: -6.53617 LUMO: 2.42726 factor:1 | 1 (-0.37348) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28558 HOMO: -6.59332 LUMO: 1.82316 factor:1 | 1 (-0.41797) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.20602 HOMO: -6.41372 LUMO: 1.77418 factor:1 | 1 (-0.33840) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92446 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-0.05684) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02356 HOMO: -6.11168 LUMO: 1.70888 factor:1 | 1 (-0.15595) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74288 HOMO: -6.44910 LUMO: 2.23405 factor:1 | -1 (0.12474) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16985 HOMO: -6.24773 LUMO: 2.12793 factor:1 | 1 (-0.30224) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44227 HOMO: -6.07358 LUMO: 1.89663 factor:1 | -1 (0.42534) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36690 HOMO: -6.66679 LUMO: 1.96738 factor:1 | -1 (0.50072) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.86376 HOMO: -6.68312 LUMO: 1.78235 factor:1 | -1 (1.00386) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15043 HOMO: -6.70761 LUMO: 1.97555 factor:1 | -1 (0.71718) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.47558 HOMO: -6.15794 LUMO: 2.00548 factor:1 | -1 (0.39203) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55945 HOMO: -6.52257 LUMO: 1.96738 factor:1 | -1 (0.30817) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74087 HOMO: -6.25590 LUMO: 1.86670 factor:1 | -1 (0.12675) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91254 HOMO: -6.30216 LUMO: 1.84765 factor:1 | 1 (-0.04493) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39217 HOMO: -6.76747 LUMO: 2.20956 factor:1 | 1 (-0.52455) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45666 HOMO: -6.14161 LUMO: 1.80684 factor:1 | 1 (-0.58904) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02263 HOMO: -6.81373 LUMO: 1.91024 factor:1 | 1 (-1.15501) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02990 HOMO: -6.81917 LUMO: 2.34834 factor:1 | 1 (-1.16228) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24746 HOMO: -6.72121 LUMO: 1.90208 factor:1 | 1 (-0.37984) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79479 HOMO: -7.51851 LUMO: 0.26939 factor:1 | 1 (-0.92717) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.49862 HOMO: -6.65318 LUMO: -0.57144 factor:1 | 1 (-0.63100) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13491 HOMO: -6.77564 LUMO: -0.72654 factor:1 | 1 (-0.26730) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.29655 HOMO: -6.80557 LUMO: -0.60954 factor:1 | 1 (-0.42893) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99883 HOMO: -7.35524 LUMO: 0.27483 factor:1 | 1 (-0.13121) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28585 HOMO: -6.94979 LUMO: -0.83811 factor:1 | 1 (-0.41824) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21506 HOMO: -6.13345 LUMO: -0.67212 factor:1 | -1 (0.65256) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29101 HOMO: -6.47359 LUMO: -0.59321 factor:1 | -1 (0.57661) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22760 HOMO: -6.52257 LUMO: -0.54695 factor:1 | -1 (0.64001) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15109 HOMO: -6.61781 LUMO: -0.69661 factor:1 | -1 (0.71653) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16891 HOMO: -6.77564 LUMO: -0.80001 factor:1 | -1 (0.69871) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.05182 HOMO: -7.35252 LUMO: -1.00410 factor:1 | -1 (0.81580) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45805 HOMO: -6.35386 LUMO: -0.38912 factor:1 | 1 (-0.59043) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.01395 HOMO: -6.80285 LUMO: -0.52246 factor:1 | 1 (-1.14633) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74042 HOMO: -7.23279 LUMO: 0.30477 factor:1 | 1 (-0.87281) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12012 HOMO: -7.13483 LUMO: -0.76192 factor:1 | -1 (0.74750) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69291 HOMO: -6.71849 LUMO: -0.48164 factor:1 | 1 (-0.82529) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39290 HOMO: -6.85455 LUMO: -0.69389 factor:1 | 1 (-0.52529) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48886 HOMO: -6.96339 LUMO: -0.73743 factor:1 | -1 (0.37876) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54763 HOMO: -7.50490 LUMO: 0.28844 factor:1 | 1 (-0.68001) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78378 HOMO: -6.63958 LUMO: -0.50069 factor:1 | -1 (0.08384) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11225 HOMO: -6.78924 LUMO: -0.69661 factor:1 | 1 (-0.24463) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15930 HOMO: -7.44776 LUMO: 0.33742 factor:1 | -1 (0.70831) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19441 HOMO: -6.15249 LUMO: 0.66396 factor:1 | -1 (0.67321) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.23299 HOMO: -6.17426 LUMO: 0.55511 factor:1 | -1 (0.63462) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.31601 HOMO: -6.83550 LUMO: 0.28844 factor:1 | -1 (0.55160) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15661 HOMO: -6.32393 LUMO: 0.47620 factor:1 | -1 (0.71101) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26423 HOMO: -6.32937 LUMO: 0.45987 factor:1 | -1 (0.60339) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38249 HOMO: -7.37429 LUMO: 0.09252 factor:1 | -1 (0.48512) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.99631 HOMO: -6.54434 LUMO: -0.39729 factor:1 | -1 (0.87131) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.27751 HOMO: -7.35524 LUMO: 0.28028 factor:1 | -1 (0.59011) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.97764 HOMO: -6.95523 LUMO: -0.86804 factor:1 | -1 (0.88998) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.18763 HOMO: -6.63958 LUMO: -0.65307 factor:1 | -1 (0.67999) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.03413 HOMO: -6.73482 LUMO: -0.67212 factor:1 | -1 (0.83348) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.14597 HOMO: -6.37835 LUMO: -0.53606 factor:1 | -1 (0.72165) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32722 HOMO: -6.71849 LUMO: -0.61226 factor:1 | -1 (0.54039) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32118 HOMO: -6.68584 LUMO: -1.11022 factor:1 | -1 (0.54643) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29762 HOMO: -6.80285 LUMO: -0.79185 factor:1 | -1 (0.57000) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.35191 HOMO: -7.14571 LUMO: -0.94696 factor:1 | -1 (0.51571) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10613 HOMO: -7.16204 LUMO: -0.66124 factor:1 | -1 (0.76148) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.99032 HOMO: -6.54978 LUMO: -0.54967 factor:1 | -1 (0.87730) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.11903 HOMO: -6.75114 LUMO: -0.70750 factor:1 | -1 (0.74859) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20641 HOMO: -7.22190 LUMO: 0.39184 factor:1 | -1 (0.66121) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.23065 HOMO: -7.43959 LUMO: 0.30477 factor:1 | -1 (0.63696) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84772 HOMO: -6.87360 LUMO: -0.77552 factor:1 | -1 (0.01989) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84225 HOMO: -6.82734 LUMO: -0.59593 factor:1 | -1 (0.02536) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95804 HOMO: -6.65318 LUMO: -0.46259 factor:1 | 1 (-0.09042) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89110 HOMO: -7.05863 LUMO: -1.17009 factor:1 | 1 (-0.02348) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32540 HOMO: -6.57427 LUMO: -0.48708 factor:1 | -1 (0.54221) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33860 HOMO: -6.60420 LUMO: -0.38096 factor:1 | -1 (0.52902) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.95103 HOMO: -6.72121 LUMO: -0.66668 factor:1 | -1 (0.91659) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20390 HOMO: -6.52257 LUMO: -0.19320 factor:1 | -1 (0.66371) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.66149 HOMO: -6.28039 LUMO: -0.27211 factor:1 | -1 (0.20613) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80655 HOMO: -6.71849 LUMO: -0.42722 factor:1 | -1 (0.06106) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.70359 HOMO: -6.27495 LUMO: 0.27756 factor:1 | -1 (0.16403) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.71211 HOMO: -6.21780 LUMO: 0.46531 factor:1 | -1 (1.15550) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.97443 HOMO: -6.52257 LUMO: -0.64491 factor:1 | -1 (0.89319) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19811 HOMO: -6.73754 LUMO: 1.83133 factor:1 | -1 (0.66951) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.99636 HOMO: -6.67223 LUMO: 1.88847 factor:1 | -1 (0.87125) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.41661 HOMO: -6.82189 LUMO: 1.59187 factor:1 | -1 (0.45100) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55313 HOMO: -6.43277 LUMO: 1.76330 factor:1 | -1 (0.31448) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53368 HOMO: -6.48175 LUMO: 1.77962 factor:1 | -1 (0.33394) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.49403 HOMO: -6.50352 LUMO: 1.68438 factor:1 | -1 (0.37359) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02609 HOMO: -6.31576 LUMO: 2.03813 factor:1 | 1 (-0.15848) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99331 HOMO: -6.27495 LUMO: 1.99459 factor:1 | 1 (-0.12569) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91513 HOMO: -6.23957 LUMO: 2.17147 factor:1 | 1 (-0.04751) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87646 HOMO: -6.78108 LUMO: 2.16875 factor:1 | 1 (-0.00884) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96890 HOMO: -6.34297 LUMO: 2.10344 factor:1 | 1 (-0.10128) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95948 HOMO: -6.30216 LUMO: 2.00004 factor:1 | 1 (-0.09187) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82661 HOMO: -6.72665 LUMO: 2.09528 factor:1 | -1 (0.04101) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37893 HOMO: -6.86543 LUMO: 1.91568 factor:1 | -1 (0.48869) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.11280 HOMO: -5.83956 LUMO: 1.89391 factor:1 | -1 (0.75482) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.23784 HOMO: -6.42189 LUMO: 2.03269 factor:1 | -1 (0.62978) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36646 HOMO: -6.07630 LUMO: 1.80956 factor:1 | -1 (0.50115) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33119 HOMO: -6.43277 LUMO: 1.81772 factor:1 | 1 (-0.46357) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36417 HOMO: -7.03959 LUMO: 1.78779 factor:1 | 1 (-0.49655) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31282 HOMO: -6.72121 LUMO: 2.29664 factor:1 | 1 (-0.44521) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57008 HOMO: -6.62869 LUMO: 2.04630 factor:1 | 1 (-0.70246) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47103 HOMO: -6.63958 LUMO: 1.84221 factor:1 | 1 (-0.60341) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55476 HOMO: -6.70761 LUMO: 1.67350 factor:1 | 1 (-0.68714) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.63914 HOMO: -6.00283 LUMO: 1.64357 factor:1 | 1 (-0.77152) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.37704 HOMO: -6.48719 LUMO: 1.70343 factor:1 | 1 (-0.50942) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08550 HOMO: -6.13345 LUMO: 1.44492 factor:1 | 1 (-0.21788) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04199 HOMO: -6.11168 LUMO: 1.70071 factor:1 | 1 (-0.17437) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15048 HOMO: -6.09535 LUMO: 1.82316 factor:1 | 1 (-0.28286) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82046 HOMO: -6.81101 LUMO: 1.63540 factor:1 | -1 (0.04716) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96307 HOMO: -6.80013 LUMO: 2.12249 factor:1 | 1 (-0.09546) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06656 HOMO: -6.48447 LUMO: 1.94561 factor:1 | 1 (-0.19894) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98599 HOMO: -6.72393 LUMO: 2.06534 factor:1 | 1 (-0.11837) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.81549 HOMO: -6.34570 LUMO: 1.98915 factor:1 | 1 (-1.94787) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10105 HOMO: -6.31304 LUMO: 1.87759 factor:1 | 1 (-1.23344) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.81864 HOMO: -6.77564 LUMO: 1.81228 factor:1 | 1 (-1.95103) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14171 HOMO: -6.58516 LUMO: 2.34834 factor:1 | 1 (-1.27409) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10149 HOMO: -6.68040 LUMO: 2.20412 factor:1 | 1 (-1.23387) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.67225 HOMO: -6.20964 LUMO: 2.17147 factor:1 | 1 (-1.80463) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23156 HOMO: -6.54706 LUMO: 2.03813 factor:1 | 1 (-1.36394) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33581 HOMO: -6.54162 LUMO: 2.17419 factor:1 | 1 (-1.46819) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.61559 HOMO: -6.75659 LUMO: 2.22589 factor:1 | 1 (-1.74798) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.99361 HOMO: -6.59604 LUMO: 2.59325 factor:1 | 1 (-2.12600) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12756 HOMO: -6.11712 LUMO: 2.02181 factor:1 | 1 (-1.25994) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05330 HOMO: -6.63141 LUMO: 2.09256 factor:1 | 1 (-1.18568) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.46797 HOMO: -6.61781 LUMO: 1.86126 factor:1 | 1 (-1.60036) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11371 HOMO: -6.63958 LUMO: 1.77146 factor:1 | 1 (-1.24609) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.67472 HOMO: -6.60420 LUMO: 1.54561 factor:1 | 1 (-1.80711) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15637 HOMO: -6.52529 LUMO: 2.05174 factor:1 | 1 (-1.28876) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18345 HOMO: -6.80285 LUMO: 2.13609 factor:1 | 1 (-1.31583) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15624 HOMO: -6.51168 LUMO: 2.25855 factor:1 | 1 (-1.28862) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96666 HOMO: -6.64774 LUMO: 2.46263 factor:1 | 1 (-1.09904) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79786 HOMO: -6.40828 LUMO: 1.99732 factor:1 | 1 (-0.93025) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06176 HOMO: -5.97562 LUMO: 1.56465 factor:1 | 1 (-1.19414) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.28400 HOMO: -6.75659 LUMO: 2.23405 factor:1 | 1 (-1.41638) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24877 HOMO: -6.68584 LUMO: 2.09528 factor:1 | 1 (-0.38115) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42425 HOMO: -6.86543 LUMO: 1.95106 factor:1 | 1 (-0.55664) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.85906 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-0.99145) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93019 HOMO: -6.87632 LUMO: 2.08439 factor:1 | 1 (-1.06258) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93368 HOMO: -6.33753 LUMO: 2.16603 factor:1 | 1 (-1.06606) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91686 HOMO: -6.92258 LUMO: 1.72248 factor:1 | 1 (-1.04924) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55544 HOMO: -6.62597 LUMO: 2.10344 factor:1 | 1 (-0.68782) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83925 HOMO: -6.63141 LUMO: 1.94017 factor:1 | 1 (-0.97164) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.86527 HOMO: -6.48447 LUMO: 1.91840 factor:1 | 1 (-0.99765) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73601 HOMO: -6.41372 LUMO: 1.61364 factor:1 | 1 (-0.86840) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.34088 HOMO: -6.37291 LUMO: 1.79051 factor:1 | 1 (-0.47326) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33318 HOMO: -6.13073 LUMO: 1.77962 factor:1 | 1 (-0.46556) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16066 HOMO: -6.13073 LUMO: 1.98915 factor:1 | 1 (-0.29304) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15519 HOMO: -6.44094 LUMO: 1.58370 factor:1 | 1 (-0.28757) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31312 HOMO: -6.87087 LUMO: -0.82995 factor:1 | 1 (-0.44550) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26166 HOMO: -6.67223 LUMO: 1.08029 factor:1 | 1 (-0.39405) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08972 HOMO: -6.82462 LUMO: 0.91702 factor:1 | 1 (-0.22210) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24419 HOMO: -6.65863 LUMO: 1.52656 factor:1 | 1 (-0.37658) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38554 HOMO: -6.78924 LUMO: 0.86260 factor:1 | -1 (0.48208) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.93339 HOMO: -6.68584 LUMO: 0.94424 factor:1 | -1 (0.93422) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09634 HOMO: -6.58788 LUMO: 1.00138 factor:1 | -1 (0.77128) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.11035 HOMO: -6.79740 LUMO: 0.91430 factor:1 | -1 (0.75727) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.98825 HOMO: -6.67223 LUMO: 0.80274 factor:1 | -1 (0.87936) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13435 HOMO: -6.95251 LUMO: 0.90614 factor:1 | -1 (0.73327) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30709 HOMO: -7.19469 LUMO: 1.34152 factor:1 | -1 (0.56053) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.08537 HOMO: -6.59332 LUMO: -0.76464 factor:1 | -1 (0.78225) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42297 HOMO: -6.77564 LUMO: -0.90886 factor:1 | 1 (-0.55536) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33984 HOMO: -6.57971 LUMO: -0.41633 factor:1 | 1 (-0.47223) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11976 HOMO: -6.68856 LUMO: -0.58232 factor:1 | 1 (-0.25214) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.85617 HOMO: -6.87087 LUMO: -0.71022 factor:1 | -1 (1.01145) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.04330 HOMO: -6.67767 LUMO: -0.74559 factor:1 | -1 (0.82431) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.07617 HOMO: -6.68040 LUMO: -0.65307 factor:1 | -1 (0.79144) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75152 HOMO: -6.32937 LUMO: 0.80274 factor:1 | 1 (-0.88391) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53432 HOMO: -6.29671 LUMO: 0.82723 factor:1 | 1 (-0.66671) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90451 HOMO: -6.67767 LUMO: 0.59321 factor:1 | 1 (-0.03690) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72589 HOMO: -6.77836 LUMO: 0.50341 factor:1 | 1 (-0.85827) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01573 HOMO: -6.61781 LUMO: 0.42450 factor:1 | 1 (-0.14811) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05162 HOMO: -6.83278 LUMO: 0.39457 factor:1 | 1 (-0.18400) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17366 HOMO: -6.56883 LUMO: 0.64219 factor:1 | 1 (-0.30605) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03652 HOMO: -6.71577 LUMO: 0.40001 factor:1 | 1 (-0.16890) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98569 HOMO: -6.86543 LUMO: -0.74287 factor:1 | 1 (-0.11807) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02408 HOMO: -6.68584 LUMO: -0.69389 factor:1 | 1 (-0.15647) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98286 HOMO: -6.61237 LUMO: -0.48980 factor:1 | 1 (-0.11524) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94084 HOMO: -6.80285 LUMO: -0.58232 factor:1 | 1 (-0.07323) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99809 HOMO: -6.88992 LUMO: -0.70205 factor:1 | 1 (-0.13048) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48807 HOMO: -6.95251 LUMO: -0.71838 factor:1 | -1 (0.37954) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99883 HOMO: -7.52123 LUMO: 0.27211 factor:1 | 1 (-0.13121) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.70652 HOMO: -6.76747 LUMO: -0.74015 factor:1 | -1 (0.16109) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96571 HOMO: -6.55250 LUMO: -0.49797 factor:1 | 1 (-0.09810) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16569 HOMO: -6.50896 LUMO: -0.46804 factor:1 | 1 (-0.29807) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57245 HOMO: -7.45320 LUMO: 0.08436 factor:1 | -1 (0.29516) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00691 HOMO: -6.82462 LUMO: -0.70477 factor:1 | 1 (-0.13930) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05717 HOMO: -6.57155 LUMO: -0.43538 factor:1 | 1 (-0.18955) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74489 HOMO: -6.72665 LUMO: -0.55239 factor:1 | -1 (0.12272) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02057 HOMO: -7.05319 LUMO: -1.08573 factor:1 | 1 (-0.15296) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74764 HOMO: -6.56067 LUMO: -0.45715 factor:1 | -1 (0.11998) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79363 HOMO: -6.76475 LUMO: -0.53879 factor:1 | -1 (0.07399) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97203 HOMO: -6.67223 LUMO: -0.45987 factor:1 | 1 (-0.10441) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36546 HOMO: -6.44094 LUMO: -0.72110 factor:1 | -1 (0.50216) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02612 HOMO: -6.66951 LUMO: -0.67756 factor:1 | 1 (-0.15851) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.56636 HOMO: -6.69400 LUMO: -0.62858 factor:1 | -1 (0.30126) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94832 HOMO: -6.51985 LUMO: -0.37007 factor:1 | 1 (-0.08071) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57482 HOMO: -5.98378 LUMO: 0.78641 factor:1 | -1 (0.29279) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77689 HOMO: -6.11440 LUMO: 0.71294 factor:1 | -1 (0.09072) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88808 HOMO: -6.45182 LUMO: 0.63947 factor:1 | 1 (-0.02046) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91505 HOMO: -6.78924 LUMO: 0.37007 factor:1 | 1 (-0.04743) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83306 HOMO: -6.63686 LUMO: 0.54423 factor:1 | -1 (0.03456) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94492 HOMO: -6.66679 LUMO: 0.48708 factor:1 | 1 (-0.07731) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36115 HOMO: -6.81917 LUMO: 0.31021 factor:1 | 1 (-0.49353) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31671 HOMO: -6.28583 LUMO: 0.44899 factor:1 | 1 (-0.44910) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30262 HOMO: -6.61237 LUMO: 0.49525 factor:1 | 1 (-0.43500) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40945 HOMO: -7.08857 LUMO: 0.38368 factor:1 | 1 (-0.54183) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17018 HOMO: -6.53890 LUMO: -0.68845 factor:1 | 1 (-0.30256) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.85122 HOMO: -6.56611 LUMO: -0.66396 factor:1 | 1 (-1.98360) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.16431 HOMO: -6.04909 LUMO: -0.59865 factor:1 | 1 (-2.29670) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.62114 HOMO: -6.74842 LUMO: -0.77825 factor:1 | 1 (-1.75353) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.94599 HOMO: -6.82462 LUMO: -0.61498 factor:1 | 1 (-2.07838) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.17431 HOMO: -7.40694 LUMO: 0.32926 factor:1 | 1 (-1.30669) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.81530 HOMO: -6.80557 LUMO: -0.57416 factor:1 | 1 (-1.94768) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52131 HOMO: -6.76747 LUMO: -0.67484 factor:1 | 1 (-1.65369) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76513 HOMO: -7.23279 LUMO: 0.48980 factor:1 | 1 (-0.89751) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.22299 HOMO: -6.62869 LUMO: -0.24762 factor:1 | 1 (-1.35537) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.85802 HOMO: -6.65863 LUMO: -0.28028 factor:1 | 1 (-1.99040) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68275 HOMO: -6.50352 LUMO: -0.44899 factor:1 | 1 (-1.81514) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94641 HOMO: -6.62053 LUMO: -0.88437 factor:1 | 1 (-1.07880) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53161 HOMO: -6.73754 LUMO: -0.77825 factor:1 | -1 (0.33601) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94811 HOMO: -7.24639 LUMO: 0.35647 factor:1 | 1 (-0.08049) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.75099 HOMO: -6.46270 LUMO: -0.48164 factor:1 | -1 (0.11663) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88724 HOMO: -6.14161 LUMO: -0.66396 factor:1 | 1 (-0.01962) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91850 HOMO: -6.63414 LUMO: 1.51295 factor:1 | 1 (-0.05089) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78230 HOMO: -6.52529 LUMO: 1.65989 factor:1 | 1 (-0.91468) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47867 HOMO: -6.63686 LUMO: 1.64629 factor:1 | 1 (-0.61106) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47038 HOMO: -6.49808 LUMO: 1.60003 factor:1 | 1 (-0.60276) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90641 HOMO: -6.85183 LUMO: 1.96194 factor:1 | 1 (-1.03879) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.66709 HOMO: -6.90081 LUMO: 1.82316 factor:1 | 1 (-0.79947) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61171 HOMO: -6.20147 LUMO: 1.95106 factor:1 | 1 (-0.74410) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79452 HOMO: -7.05047 LUMO: 1.94289 factor:1 | 1 (-0.92690) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.61153 HOMO: -6.11440 LUMO: 1.83949 factor:1 | -1 (0.25609) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.67482 HOMO: -6.65046 LUMO: 1.59187 factor:1 | -1 (0.19279) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85953 HOMO: -6.81917 LUMO: 2.41365 factor:1 | -1 (0.00808) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01194 HOMO: -6.40284 LUMO: 2.48984 factor:1 | 1 (-0.14433) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91330 HOMO: -7.04775 LUMO: 2.31025 factor:1 | 1 (-0.04569) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65793 HOMO: -6.64774 LUMO: 2.20140 factor:1 | 1 (-1.79032) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.59562 HOMO: -6.72393 LUMO: 2.28304 factor:1 | 1 (-1.72800) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03224 HOMO: -6.35114 LUMO: 1.84765 factor:1 | 1 (-1.16462) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.41910 HOMO: -6.41100 LUMO: 1.74697 factor:1 | 1 (-1.55148) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70148 HOMO: -6.34297 LUMO: 1.55921 factor:1 | 1 (-0.83387) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79781 HOMO: -6.31848 LUMO: 1.67622 factor:1 | 1 (-0.93019) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94813 HOMO: -6.50896 LUMO: 2.02725 factor:1 | 1 (-1.08051) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.81092 HOMO: -6.28583 LUMO: 2.00548 factor:1 | 1 (-1.94330) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06168 HOMO: -6.67495 LUMO: 1.92384 factor:1 | 1 (-1.19406) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14097 HOMO: -6.17154 LUMO: 2.39732 factor:1 | 1 (-1.27336) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10179 HOMO: -6.84911 LUMO: 2.24766 factor:1 | 1 (-1.23417) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17042 HOMO: -6.77564 LUMO: 2.38372 factor:1 | 1 (-0.30281) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13732 HOMO: -6.18243 LUMO: 2.40821 factor:1 | -1 (0.73030) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.50277 HOMO: -6.40828 LUMO: 2.22589 factor:1 | -1 (0.36485) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52027 HOMO: -6.74570 LUMO: 1.88303 factor:1 | 1 (-1.65266) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15556 HOMO: -6.29944 LUMO: 2.05174 factor:1 | 1 (-1.28794) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.35782 HOMO: -7.00693 LUMO: 2.16331 factor:1 | 1 (-1.49020) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.02450 HOMO: -6.89537 LUMO: 2.19596 factor:1 | 1 (-2.15688) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.15536 HOMO: -6.72665 LUMO: 2.03813 factor:1 | 1 (-2.28774) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.31681 HOMO: -6.69944 LUMO: 2.36467 factor:1 | 1 (-1.44920) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37877 HOMO: -6.92802 LUMO: 1.72792 factor:1 | 1 (-1.51116) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.07528 HOMO: -6.12256 LUMO: 1.85310 factor:1 | 1 (-2.20766) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.98181 HOMO: -6.70489 LUMO: 2.20956 factor:1 | 1 (-1.11420) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45835 HOMO: -6.94707 LUMO: 1.81500 factor:1 | 1 (-0.59073) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15839 HOMO: -6.39468 LUMO: 1.79051 factor:1 | 1 (-1.29077) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27725 HOMO: -6.69128 LUMO: 2.03813 factor:1 | 1 (-1.40963) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08313 HOMO: -6.55250 LUMO: 2.00548 factor:1 | 1 (-0.21551) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14830 HOMO: -6.24773 LUMO: 2.09256 factor:1 | 1 (-0.28069) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.52787 HOMO: -6.85727 LUMO: 1.70071 factor:1 | 1 (-0.66026) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39146 HOMO: -6.71305 LUMO: 1.72520 factor:1 | 1 (-0.52385) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.34571 HOMO: -6.81101 LUMO: 2.15514 factor:1 | 1 (-1.47810) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.16693 HOMO: -6.93618 LUMO: 1.75513 factor:1 | 1 (-1.29932) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.21494 HOMO: -6.63686 LUMO: 2.09800 factor:1 | 1 (-0.34733) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09570 HOMO: -6.98244 LUMO: 1.72520 factor:1 | 1 (-0.22809) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59313 HOMO: -6.37019 LUMO: 2.35923 factor:1 | 1 (-0.72551) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99498 HOMO: -6.55794 LUMO: 2.12521 factor:1 | 1 (-1.12737) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.00913 HOMO: -6.45998 LUMO: 1.93201 factor:1 | 1 (-1.14152) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96471 HOMO: -6.71033 LUMO: 1.58370 factor:1 | 1 (-0.09709) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94299 HOMO: -6.67223 LUMO: 1.52928 factor:1 | 1 (-0.07538) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22400 HOMO: -6.72121 LUMO: 1.33608 factor:1 | 1 (-0.35639) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.21015 HOMO: -6.89264 LUMO: 2.08983 factor:1 | 1 (-0.34254) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.64408 HOMO: -6.31032 LUMO: 2.24766 factor:1 | 1 (-1.77647) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.37887 HOMO: -6.79740 LUMO: 2.09528 factor:1 | 1 (-2.51126) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.28065 HOMO: -6.78108 LUMO: 2.15786 factor:1 | 1 (-1.41303) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07556 HOMO: -6.50896 LUMO: 2.15786 factor:1 | 1 (-1.20794) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95107 HOMO: -6.56067 LUMO: 2.24494 factor:1 | 1 (-0.08346) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58526 HOMO: -6.72938 LUMO: 2.24494 factor:1 | 1 (-0.71765) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30224 HOMO: -6.40556 LUMO: 1.58642 factor:1 | 1 (-0.43462) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97409 HOMO: -6.63141 LUMO: 1.66262 factor:1 | 1 (-1.10647) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.82273 HOMO: -6.97156 LUMO: 2.23678 factor:1 | 1 (-1.95511) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.02009 HOMO: -6.86271 LUMO: 1.91296 factor:1 | 1 (-2.15248) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.11304 HOMO: -6.50624 LUMO: 1.89119 factor:1 | 1 (-2.24543) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06726 HOMO: -6.70761 LUMO: 1.56193 factor:1 | 1 (-1.19964) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33668 HOMO: -6.60420 LUMO: 1.79595 factor:1 | 1 (-1.46906) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02990 HOMO: -6.85727 LUMO: 2.26943 factor:1 | 1 (-1.16228) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25020 HOMO: -6.23413 LUMO: 1.91024 factor:1 | 1 (-1.38258) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88233 HOMO: -6.84366 LUMO: 2.01364 factor:1 | 1 (-1.01471) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80674 HOMO: -6.63414 LUMO: 2.54971 factor:1 | 1 (-0.93912) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.04570 HOMO: -6.52257 LUMO: 2.42998 factor:1 | -1 (0.82192) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.18121 HOMO: -6.61509 LUMO: 2.31297 factor:1 | -1 (0.68641) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.05454 HOMO: -6.45998 LUMO: 2.23405 factor:1 | -1 (0.81308) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30140 HOMO: -6.86271 LUMO: 2.22317 factor:1 | -1 (0.56621) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03896 HOMO: -6.84366 LUMO: 2.11432 factor:1 | 1 (-1.17134) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23322 HOMO: -6.85999 LUMO: 2.44902 factor:1 | 1 (-1.36560) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92611 HOMO: -6.73482 LUMO: 1.93745 factor:1 | 1 (-1.05850) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88059 HOMO: -6.91441 LUMO: 2.32385 factor:1 | 1 (-1.01297) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.01141 HOMO: -6.16066 LUMO: 2.26399 factor:1 | -1 (0.85621) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15441 HOMO: -6.71305 LUMO: 2.38644 factor:1 | -1 (0.71321) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27186 HOMO: -7.08312 LUMO: 2.01636 factor:1 | 1 (-1.40424) | 1 | 1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.21145 HOMO: -6.15249 LUMO: 1.90752 factor:1 | 1 (-1.34383) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11469 HOMO: -6.83006 LUMO: 2.25855 factor:1 | 1 (-1.24707) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83855 HOMO: -6.77836 LUMO: 2.24766 factor:1 | -1 (0.02906) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.70889 HOMO: -6.66951 LUMO: 2.35923 factor:1 | -1 (0.15872) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89654 HOMO: -6.68312 LUMO: 2.30208 factor:1 | 1 (-0.02893) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.57785 HOMO: -6.49808 LUMO: 2.49801 factor:1 | 1 (-1.71024) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90206 HOMO: -6.62325 LUMO: 1.89935 factor:1 | 1 (-1.03444) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75936 HOMO: -6.80829 LUMO: 1.91296 factor:1 | 1 (-0.89174) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89466 HOMO: -6.64230 LUMO: 2.13065 factor:1 | 1 (-1.02704) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.10557 HOMO: -6.40556 LUMO: 1.83949 factor:1 | -1 (1.76205) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.36568 HOMO: -6.48175 LUMO: 1.72248 factor:1 | -1 (1.50193) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.64373 HOMO: -6.61781 LUMO: 2.11432 factor:1 | -1 (1.22389) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.79271 HOMO: -6.34570 LUMO: 2.22317 factor:1 | -1 (1.07490) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.46887 HOMO: -7.00149 LUMO: 1.80139 factor:1 | 1 (-1.60125) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25186 HOMO: -6.66951 LUMO: 2.13065 factor:1 | 1 (-1.38424) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.49655 HOMO: -6.54434 LUMO: 2.20140 factor:1 | 1 (-0.62894) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72434 HOMO: -6.67767 LUMO: 2.02997 factor:1 | 1 (-0.85672) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17061 HOMO: -6.49536 LUMO: 2.42998 factor:1 | 1 (-0.30300) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99692 HOMO: -6.70761 LUMO: 2.71025 factor:1 | 1 (-0.12931) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05535 HOMO: -6.62869 LUMO: 2.11160 factor:1 | 1 (-0.18773) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18830 HOMO: -6.61781 LUMO: 2.24494 factor:1 | 1 (-0.32069) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.99957 HOMO: -6.66135 LUMO: 2.20956 factor:1 | -1 (0.86804) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26975 HOMO: -6.95523 LUMO: 2.03813 factor:1 | -1 (0.59786) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23088 HOMO: -7.11578 LUMO: 2.41365 factor:1 | 1 (-1.36326) | 1 | 1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46009 HOMO: -6.99061 LUMO: 2.13881 factor:1 | 1 (-0.59247) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33630 HOMO: -6.43277 LUMO: 2.01364 factor:1 | 1 (-1.46868) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18535 HOMO: -6.79196 LUMO: 2.04358 factor:1 | 1 (-1.31774) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.00753 HOMO: -7.08584 LUMO: 1.99732 factor:1 | 1 (-1.13991) | 1 | 1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23905 HOMO: -6.46815 LUMO: 2.29936 factor:1 | 1 (-0.37144) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.37549 HOMO: -6.78108 LUMO: 1.93745 factor:1 | 1 (-0.50787) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57008 HOMO: -6.43277 LUMO: 1.80956 factor:1 | 1 (-0.70246) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42923 HOMO: -6.71577 LUMO: -0.81090 factor:1 | 1 (-0.56162) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17105 HOMO: -7.14027 LUMO: -0.68028 factor:1 | 1 (-0.30343) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.83919 HOMO: -7.03414 LUMO: -0.69661 factor:1 | -1 (1.02843) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.02872 HOMO: -6.64502 LUMO: -0.47348 factor:1 | -1 (0.83890) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31766 HOMO: -6.60692 LUMO: 2.12793 factor:1 | 1 (-0.45005) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14944 HOMO: -6.66407 LUMO: 1.94561 factor:1 | 1 (-0.28183) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03649 HOMO: -7.10217 LUMO: 1.92384 factor:1 | 1 (-0.16887) | 1 | 1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99426 HOMO: -6.84094 LUMO: 1.66534 factor:1 | 1 (-0.12664) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.20757 HOMO: -6.93618 LUMO: 2.13065 factor:1 | 1 (-0.33995) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45184 HOMO: -6.60692 LUMO: 2.20684 factor:1 | 1 (-0.58423) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86383 HOMO: -6.85727 LUMO: 2.19324 factor:1 | -1 (0.00378) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62641 HOMO: -6.31032 LUMO: 1.76330 factor:1 | 1 (-0.75879) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04136 HOMO: -6.43821 LUMO: 2.10072 factor:1 | 1 (-0.17374) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89396 HOMO: -6.42189 LUMO: 2.19596 factor:1 | 1 (-0.02634) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87956 HOMO: -6.40556 LUMO: 2.02181 factor:1 | 1 (-0.01195) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74685 HOMO: -6.41372 LUMO: 2.26671 factor:1 | -1 (0.12076) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11048 HOMO: -6.60692 LUMO: 2.09800 factor:1 | 1 (-0.24286) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92008 HOMO: -6.75931 LUMO: 1.76602 factor:1 | 1 (-0.05246) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.29246 HOMO: -6.39195 LUMO: 1.84221 factor:1 | -1 (1.57516) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.59088 HOMO: -6.74570 LUMO: 2.04085 factor:1 | -1 (1.27673) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.75350 HOMO: -6.77019 LUMO: 2.16875 factor:1 | -1 (1.11412) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.05816 HOMO: -6.15522 LUMO: 1.81772 factor:1 | -1 (0.80946) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.08387 HOMO: -6.48175 LUMO: 2.02453 factor:1 | -1 (0.78374) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34791 HOMO: -6.57427 LUMO: 1.77962 factor:1 | -1 (0.51971) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09821 HOMO: -6.57699 LUMO: 2.42998 factor:1 | -1 (0.76940) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37014 HOMO: -6.35386 LUMO: 2.25310 factor:1 | -1 (0.49748) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44614 HOMO: -6.80013 LUMO: 2.11160 factor:1 | -1 (0.42148) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.67820 HOMO: -6.24229 LUMO: 2.05718 factor:1 | -1 (0.18942) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.69325 HOMO: -6.42733 LUMO: 1.76874 factor:1 | -1 (0.17437) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92819 HOMO: -6.56883 LUMO: 2.36195 factor:1 | 1 (-0.06057) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.80697 HOMO: -6.72665 LUMO: 2.28848 factor:1 | -1 (1.06065) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.70365 HOMO: -6.39195 LUMO: 1.79051 factor:1 | -1 (1.16397) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.75872 HOMO: -6.70761 LUMO: 0.15510 factor:1 | -1 (1.10889) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91021 HOMO: -6.44366 LUMO: -0.16871 factor:1 | -1 (0.95741) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.02940 HOMO: -6.68584 LUMO: 1.69527 factor:1 | -1 (0.83822) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.89122 HOMO: -6.26950 LUMO: 1.61636 factor:1 | -1 (0.97640) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12426 HOMO: -6.47631 LUMO: 1.98915 factor:1 | -1 (0.74336) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97352 HOMO: -6.58243 LUMO: 1.97283 factor:1 | 1 (-0.10591) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86049 HOMO: -6.51713 LUMO: 1.97283 factor:1 | -1 (0.00713) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10727 HOMO: -6.65046 LUMO: 1.69255 factor:1 | 1 (-0.23965) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37491 HOMO: -6.26406 LUMO: 2.21773 factor:1 | 1 (-1.50729) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27629 HOMO: -6.88992 LUMO: 2.28304 factor:1 | 1 (-1.40868) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42344 HOMO: -6.67767 LUMO: 2.34834 factor:1 | 1 (-0.55582) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.08786 HOMO: -6.52801 LUMO: 2.10344 factor:1 | 1 (-1.22024) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24036 HOMO: -6.52801 LUMO: 2.24222 factor:1 | 1 (-0.37274) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50534 HOMO: -6.17154 LUMO: 1.89663 factor:1 | 1 (-0.63773) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.14429 HOMO: -6.42733 LUMO: 2.15514 factor:1 | -1 (1.72332) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.01264 HOMO: -6.36474 LUMO: 2.01364 factor:1 | -1 (1.85497) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.21159 HOMO: -6.82189 LUMO: 1.86942 factor:1 | -1 (1.65603) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13277 HOMO: -6.60148 LUMO: 2.00548 factor:1 | -1 (0.73484) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.95255 HOMO: -6.67767 LUMO: 2.15786 factor:1 | -1 (0.91506) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16126 HOMO: -6.79196 LUMO: 2.06534 factor:1 | -1 (0.70635) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.80066 HOMO: -6.70216 LUMO: 1.83405 factor:1 | -1 (1.06696) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.61755 HOMO: -6.58788 LUMO: 1.79051 factor:1 | -1 (1.25006) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.84907 HOMO: -6.34842 LUMO: 1.80139 factor:1 | -1 (1.01855) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39076 HOMO: -6.48175 LUMO: 1.95922 factor:1 | -1 (0.47685) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32137 HOMO: -6.71033 LUMO: 2.02997 factor:1 | -1 (0.54624) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55460 HOMO: -6.89264 LUMO: 2.42726 factor:1 | -1 (0.31301) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.36911 HOMO: -6.74570 LUMO: 2.20684 factor:1 | 1 (-1.50150) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.38422 HOMO: -6.30216 LUMO: 2.15242 factor:1 | 1 (-1.51660) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45623 HOMO: -6.94979 LUMO: 2.43814 factor:1 | 1 (-0.58861) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27794 HOMO: -6.97972 LUMO: 2.11432 factor:1 | 1 (-0.41032) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.09567 HOMO: -6.17154 LUMO: 1.98099 factor:1 | 1 (-1.22805) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45756 HOMO: -6.74026 LUMO: 2.21501 factor:1 | 1 (-0.58994) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53059 HOMO: -6.72393 LUMO: 2.19596 factor:1 | 1 (-0.66298) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38134 HOMO: -6.11440 LUMO: 2.10072 factor:1 | 1 (-0.51372) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28365 HOMO: -6.34297 LUMO: 1.92657 factor:1 | 1 (-0.41603) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25554 HOMO: -6.24773 LUMO: 2.00276 factor:1 | 1 (-0.38793) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50651 HOMO: -6.75114 LUMO: 1.98643 factor:1 | 1 (-0.63890) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90781 HOMO: -6.69128 LUMO: 2.08711 factor:1 | 1 (-0.04019) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15015 HOMO: -6.65318 LUMO: 2.15514 factor:1 | 1 (-0.28254) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33560 HOMO: -6.67495 LUMO: 1.72248 factor:1 | 1 (-0.46798) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22896 HOMO: -6.58243 LUMO: 1.83405 factor:1 | 1 (-0.36134) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03801 HOMO: -6.61237 LUMO: 1.69799 factor:1 | 1 (-0.17040) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05872 HOMO: -6.57427 LUMO: 2.29936 factor:1 | 1 (-0.19111) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27976 HOMO: -6.40012 LUMO: 2.35378 factor:1 | 1 (-0.41214) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.86379 HOMO: -6.90081 LUMO: 2.26671 factor:1 | -1 (1.00383) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.14265 HOMO: -6.44910 LUMO: 2.25855 factor:1 | -1 (0.72497) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38501 HOMO: -6.61509 LUMO: 2.26943 factor:1 | 1 (-0.51740) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10787 HOMO: -6.78924 LUMO: 2.09256 factor:1 | 1 (-0.24025) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.81818 HOMO: -6.47087 LUMO: 1.97555 factor:1 | -1 (1.04943) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.07549 HOMO: -6.75931 LUMO: 1.98643 factor:1 | -1 (0.79212) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40327 HOMO: -6.17971 LUMO: 2.09800 factor:1 | 1 (-0.53566) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32507 HOMO: -6.83006 LUMO: 1.91840 factor:1 | 1 (-0.45745) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.81493 HOMO: -6.72938 LUMO: 2.17419 factor:1 | -1 (0.05268) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53266 HOMO: -6.78924 LUMO: 2.42726 factor:1 | 1 (-0.66505) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08729 HOMO: -6.41372 LUMO: 1.93745 factor:1 | 1 (-0.21968) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.66033 HOMO: -6.85455 LUMO: 2.14970 factor:1 | -1 (1.20729) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91783 HOMO: -6.38651 LUMO: 2.18507 factor:1 | -1 (0.94979) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.73048 HOMO: -6.81373 LUMO: 2.00548 factor:1 | -1 (1.13714) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.97043 HOMO: -6.64774 LUMO: 2.41365 factor:1 | -1 (0.89719) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46992 HOMO: -6.70489 LUMO: 2.31569 factor:1 | -1 (0.39769) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.75706 HOMO: -6.49264 LUMO: 1.78779 factor:1 | -1 (0.11056) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.84675 HOMO: -6.81101 LUMO: 1.86670 factor:1 | -1 (1.02086) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10099 HOMO: -6.72121 LUMO: 1.48846 factor:1 | -1 (0.76663) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.34127 HOMO: -6.35930 LUMO: 1.78507 factor:1 | 1 (-2.47365) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.98145 HOMO: -6.38651 LUMO: 2.04358 factor:1 | 1 (-2.11383) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.31891 HOMO: -6.42189 LUMO: 1.99187 factor:1 | 1 (-1.45129) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.14771 HOMO: -6.69400 LUMO: 1.61091 factor:1 | 1 (-2.28010) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.76460 HOMO: -6.81101 LUMO: 2.17419 factor:1 | 1 (-1.89699) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81716 HOMO: -6.90897 LUMO: 2.28576 factor:1 | 1 (-0.94954) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68678 HOMO: -6.75387 LUMO: 2.31297 factor:1 | 1 (-1.81916) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.61774 HOMO: -7.05863 LUMO: 2.18780 factor:1 | 1 (-1.75013) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02971 HOMO: -6.56611 LUMO: 1.99187 factor:1 | 1 (-1.16209) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.90327 HOMO: -6.59060 LUMO: 1.86398 factor:1 | 1 (-2.03566) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.77100 HOMO: -6.59060 LUMO: 1.59459 factor:1 | 1 (-1.90338) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.88629 HOMO: -6.57699 LUMO: 1.48030 factor:1 | -1 (0.98132) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13128 HOMO: -6.99605 LUMO: 2.30208 factor:1 | -1 (0.73634) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98792 HOMO: -6.42189 LUMO: 2.20412 factor:1 | 1 (-0.12030) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78190 HOMO: -7.15115 LUMO: 1.83405 factor:1 | -1 (0.08572) | 1 | 1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.75093 HOMO: -7.08040 LUMO: 2.21773 factor:1 | -1 (0.11668) | 1 | 1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88136 HOMO: -6.72121 LUMO: 1.89663 factor:1 | 1 (-0.01374) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01156 HOMO: -6.25590 LUMO: 1.85037 factor:1 | 1 (-0.14395) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94299 HOMO: -6.70489 LUMO: 1.98915 factor:1 | 1 (-0.07538) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.67063 HOMO: -6.53617 LUMO: 2.08439 factor:1 | -1 (0.19698) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89306 HOMO: -6.69944 LUMO: 1.98915 factor:1 | 1 (-0.02544) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.84828 HOMO: -6.79468 LUMO: 1.96466 factor:1 | 1 (-1.98066) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68161 HOMO: -6.79468 LUMO: 1.99459 factor:1 | 1 (-1.81399) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79746 HOMO: -6.58788 LUMO: 1.98371 factor:1 | 1 (-0.92984) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15145 HOMO: -6.58788 LUMO: 2.16603 factor:1 | 1 (-1.28383) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52256 HOMO: -6.56883 LUMO: 1.64085 factor:1 | 1 (-1.65494) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76129 HOMO: -7.19197 LUMO: 2.66127 factor:1 | 1 (-0.89368) | 1 | 1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.77384 HOMO: -6.48175 LUMO: 2.40004 factor:1 | 1 (-0.90622) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.81040 HOMO: -6.18515 LUMO: 2.27759 factor:1 | 1 (-1.94278) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94413 HOMO: -6.64774 LUMO: 2.13337 factor:1 | 1 (-1.07651) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03934 HOMO: -6.39740 LUMO: 1.95106 factor:1 | 1 (-1.17172) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.51037 HOMO: -6.59332 LUMO: 1.81772 factor:1 | 1 (-1.64275) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.12788 HOMO: -6.68312 LUMO: 2.41909 factor:1 | 1 (-2.26026) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.28857 HOMO: -5.87494 LUMO: 2.18235 factor:1 | 1 (-1.42095) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30386 HOMO: -6.30488 LUMO: 2.04902 factor:1 | 1 (-1.43624) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96102 HOMO: -6.65046 LUMO: 2.05446 factor:1 | 1 (-1.09341) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00833 HOMO: -6.55794 LUMO: 2.06807 factor:1 | 1 (-0.14071) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97325 HOMO: -6.68040 LUMO: 1.99187 factor:1 | 1 (-0.10563) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24030 HOMO: -6.60965 LUMO: 2.18780 factor:1 | 1 (-0.37269) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18701 HOMO: -6.88176 LUMO: 2.10344 factor:1 | 1 (-1.31940) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.05171 HOMO: -6.63414 LUMO: 1.70615 factor:1 | 1 (-2.18409) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99575 HOMO: -7.15115 LUMO: 2.07351 factor:1 | 1 (-1.12813) | 1 | 1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07961 HOMO: -6.85727 LUMO: 2.27759 factor:1 | 1 (-1.21200) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27502 HOMO: -6.91713 LUMO: 2.28848 factor:1 | 1 (-1.40740) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.82293 HOMO: -7.10217 LUMO: 2.14698 factor:1 | 1 (-0.95531) | 1 | 1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90540 HOMO: -6.78108 LUMO: 2.45447 factor:1 | 1 (-1.03779) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65819 HOMO: -6.78380 LUMO: 2.43542 factor:1 | 1 (-0.79057) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93803 HOMO: -6.60965 LUMO: 2.33474 factor:1 | 1 (-1.07041) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.94670 HOMO: -6.72665 LUMO: 2.25855 factor:1 | -1 (0.92091) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98092 HOMO: -6.27495 LUMO: 2.04358 factor:1 | 1 (-0.11331) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92179 HOMO: -6.17426 LUMO: 1.45853 factor:1 | 1 (-0.05418) | -1 | -1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12169 HOMO: -7.21374 LUMO: 2.33474 factor:1 | 1 (-0.25407) | 1 | 1 |
| G: -6257.50192 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09069 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-0.22308) | -1 | -1 |
| G: -6257.50192 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.69178 HOMO: -6.80829 LUMO: 0.17960 factor:1 | -1 (1.17583) | -1 | -1 |
| G: -6257.50192 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.09286 HOMO: -7.19469 LUMO: 1.60819 factor:1 | -1 (1.77475) | 1 | 1 |
| G: -6257.50192 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.62977 HOMO: -6.78652 LUMO: 0.53334 factor:1 | -1 (1.23785) | -1 | -1 |
| G: -6257.50192 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24198 HOMO: -6.70489 LUMO: 0.74559 factor:1 | 1 (-1.37437) | -1 | -1 |
| G: -6257.50192 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14054 HOMO: -6.72393 LUMO: 0.88981 factor:1 | 1 (-1.27292) | -1 | -1 |
| G: -6257.50192 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.34397 HOMO: -4.54430 LUMO: -0.90614 factor:1 | 1 (-1.47635) | -1 | -1 |
| G: -6257.50192 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41889 HOMO: -6.83006 LUMO: 0.47348 factor:1 | 1 (-0.55128) | -1 | -1 |
| G: -6257.50192 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94424 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-0.07663) | -1 | -1 |
| G: -6257.50192 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86000 HOMO: -6.62053 LUMO: 0.74559 factor:1 | -1 (0.00762) | -1 | -1 |
| G: -6257.50192 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07510 HOMO: -6.79196 LUMO: 1.80139 factor:1 | 1 (-0.20749) | -1 | -1 |
| G: -6257.50192 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02215 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-0.15453) | -1 | -1 |
| G: -6257.50192 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.88988 HOMO: -6.74026 LUMO: 0.95784 factor:1 | -1 (0.97773) | -1 | -1 |
| G: -6257.50192 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05395 HOMO: -7.34707 LUMO: 0.40001 factor:1 | 1 (-1.18633) | -1 | -1 |
| G: -6257.50192 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14029 HOMO: -6.19875 LUMO: -0.88709 factor:1 | 1 (-1.27268) | -1 | -1 |
| G: -6257.50192 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19355 HOMO: -6.48719 LUMO: -0.14694 factor:1 | 1 (-0.32594) | -1 | -1 |
| G: -6257.50192 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99779 HOMO: -6.73482 LUMO: -0.01633 factor:1 | 1 (-1.13017) | -1 | -1 |
| G: -6257.50192 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11897 HOMO: -7.05591 LUMO: -0.20136 factor:1 | 1 (-0.25135) | -1 | -1 |
| G: -6257.50192 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18685 HOMO: -6.38651 LUMO: -2.07895 factor:1 | 1 (-1.31924) | -1 | -1 |
| G: -6257.50192 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31968 HOMO: -6.85455 LUMO: -1.03403 factor:1 | 1 (-0.45206) | -1 | -1 |
| G: -6257.50192 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33777 HOMO: -6.72121 LUMO: -0.99322 factor:1 | 1 (-0.47016) | -1 | -1 |
| G: -6257.50192 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41903 HOMO: -6.53890 LUMO: -0.10885 factor:1 | 1 (-0.55141) | -1 | -1 |
| G: -6257.50192 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09549 HOMO: -6.68312 LUMO: 0.21225 factor:1 | -1 (0.77212) | -1 | -1 |
| G: -6257.50192 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.74199 HOMO: -6.68040 LUMO: 0.21225 factor:1 | 1 (-1.87437) | -1 | -1 |
| G: -6257.50192 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.86366 HOMO: -6.76475 LUMO: -0.64491 factor:1 | 1 (-0.99605) | -1 | -1 |
| G: -6257.50192 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.04625 HOMO: -6.48175 LUMO: 0.41633 factor:1 | 1 (-1.17863) | -1 | -1 |
| G: -6257.50192 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90731 HOMO: -6.42733 LUMO: 0.16599 factor:1 | 1 (-1.03969) | -1 | -1 |
| G: -6257.50192 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10924 HOMO: -6.66679 LUMO: 0.77825 factor:1 | 1 (-1.24163) | -1 | -1 |
| G: -6257.50192 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.01285 HOMO: -6.75931 LUMO: -0.73471 factor:1 | -1 (0.85476) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83319 HOMO: -6.53617 LUMO: 0.38096 factor:1 | 1 (-1.37646) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90577 HOMO: -6.34297 LUMO: 0.35375 factor:1 | 1 (-1.44903) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.81143 HOMO: -7.11850 LUMO: -0.03265 factor:1 | 1 (-0.35470) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.76632 HOMO: -5.21914 LUMO: 1.29798 factor:1 | 1 (-0.30958) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.79222 HOMO: -7.09129 LUMO: -0.66668 factor:1 | 1 (-0.33549) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52764 HOMO: -6.96884 LUMO: -0.31021 factor:1 | 1 (-1.07090) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26042 HOMO: -6.51713 LUMO: -0.59865 factor:1 | 1 (-0.80369) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79540 HOMO: -6.69400 LUMO: -0.07075 factor:1 | 1 (-1.33866) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37977 HOMO: -5.28173 LUMO: 1.17281 factor:1 | 1 (-0.92304) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89148 HOMO: -6.54434 LUMO: 0.32109 factor:1 | 1 (-1.43475) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89268 HOMO: -6.79740 LUMO: -0.24762 factor:1 | 1 (-1.43594) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.73235 HOMO: -6.91986 LUMO: -0.14694 factor:1 | 1 (-1.27562) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85232 HOMO: -6.75114 LUMO: 0.18504 factor:1 | 1 (-1.39559) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83923 HOMO: -6.74842 LUMO: 0.69389 factor:1 | 1 (-1.38250) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.54867 HOMO: -7.01782 LUMO: 0.56600 factor:1 | 1 (-1.09194) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84936 HOMO: -6.47359 LUMO: -0.56600 factor:1 | 1 (-1.39262) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.63082 HOMO: -6.63686 LUMO: -0.55783 factor:1 | 1 (-1.17409) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77570 HOMO: -4.13885 LUMO: -2.05446 factor:1 | 1 (-1.31896) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90125 HOMO: -6.34570 LUMO: 0.19864 factor:1 | 1 (-1.44452) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91543 HOMO: -6.47903 LUMO: 0.24762 factor:1 | 1 (-1.45869) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90963 HOMO: -6.15249 LUMO: 0.32109 factor:1 | 1 (-1.45290) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.70187 HOMO: -6.84366 LUMO: 0.29116 factor:1 | 1 (-1.24514) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78941 HOMO: -6.34297 LUMO: 0.19864 factor:1 | 1 (-1.33268) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56812 HOMO: -6.51168 LUMO: 0.30749 factor:1 | 1 (-2.11139) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50893 HOMO: -6.79468 LUMO: -0.16599 factor:1 | 1 (-2.05220) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55459 HOMO: -7.24095 LUMO: 0.15238 factor:1 | 1 (-2.09786) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59323 HOMO: -7.06952 LUMO: -0.34558 factor:1 | 1 (-2.13650) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44588 HOMO: -6.88176 LUMO: 0.02177 factor:1 | 1 (-1.98915) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45884 HOMO: -6.37291 LUMO: -0.69117 factor:1 | 1 (-2.00210) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18817 HOMO: -6.83278 LUMO: -0.59049 factor:1 | 1 (-1.73143) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36762 HOMO: -6.57155 LUMO: -0.33470 factor:1 | 1 (-1.91089) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61168 HOMO: -6.89537 LUMO: -0.58504 factor:1 | 1 (-2.15495) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.49402 HOMO: -6.57155 LUMO: -0.34831 factor:1 | 1 (-2.03729) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35258 HOMO: -6.64774 LUMO: -0.95784 factor:1 | 1 (-1.89584) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32752 HOMO: -6.91713 LUMO: -0.69933 factor:1 | 1 (-1.87078) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39737 HOMO: -6.80557 LUMO: -0.65035 factor:1 | 1 (-1.94063) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41280 HOMO: -7.26544 LUMO: -0.79729 factor:1 | 1 (-1.95606) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12716 HOMO: -6.69128 LUMO: -0.16871 factor:1 | 1 (-1.67043) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31497 HOMO: -6.88448 LUMO: 0.13061 factor:1 | 1 (-1.85824) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90392 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-1.44718) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.67308 HOMO: -6.56067 LUMO: 0.17687 factor:1 | 1 (-1.21635) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78808 HOMO: -6.70216 LUMO: 0.25034 factor:1 | 1 (-1.33134) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57552 HOMO: -6.51713 LUMO: -0.78369 factor:1 | 1 (-2.11879) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68622 HOMO: -6.50352 LUMO: 0.12245 factor:1 | 1 (-2.22948) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.38402 HOMO: -6.22052 LUMO: -0.83811 factor:1 | 1 (-2.92729) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30242 HOMO: -6.51168 LUMO: -0.76464 factor:1 | 1 (-2.84569) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69574 HOMO: -7.14571 LUMO: -0.80274 factor:1 | 1 (-2.23901) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.32936 HOMO: -6.66679 LUMO: -0.88709 factor:1 | 1 (-2.87262) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31957 HOMO: -6.76203 LUMO: -1.43948 factor:1 | 1 (-1.86284) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81588 HOMO: -6.57427 LUMO: -1.62996 factor:1 | 1 (-2.35915) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06478 HOMO: -5.05043 LUMO: 1.24900 factor:1 | 1 (-2.60805) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50357 HOMO: -6.53345 LUMO: 0.23130 factor:1 | 1 (-2.04684) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.73511 HOMO: -7.18381 LUMO: -0.22585 factor:1 | 1 (-3.27837) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69759 HOMO: -7.00965 LUMO: -1.79595 factor:1 | 1 (-2.24086) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50123 HOMO: -6.08174 LUMO: -0.82995 factor:1 | 1 (-2.04450) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.63628 HOMO: -6.42189 LUMO: -0.84355 factor:1 | 1 (-2.17955) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47897 HOMO: -6.53890 LUMO: 0.60409 factor:1 | 1 (-2.02224) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35878 HOMO: -6.62869 LUMO: 0.43810 factor:1 | 1 (-1.90205) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65881 HOMO: -6.68312 LUMO: 0.64491 factor:1 | 1 (-2.20208) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91561 HOMO: -6.42189 LUMO: 1.51295 factor:1 | 1 (-2.45888) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69462 HOMO: -6.17971 LUMO: 1.67622 factor:1 | 1 (-2.23789) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78622 HOMO: -6.79196 LUMO: 1.36873 factor:1 | 1 (-2.32949) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99569 HOMO: -7.38517 LUMO: 0.56328 factor:1 | 1 (-2.53896) | 1 | 1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.66808 HOMO: -7.56204 LUMO: 0.71566 factor:1 | 1 (-3.21135) | 1 | 1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.46773 HOMO: -6.45726 LUMO: -1.91840 factor:1 | 1 (-3.01099) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.50604 HOMO: -6.13073 LUMO: -0.97417 factor:1 | 1 (-3.04931) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81286 HOMO: -6.50352 LUMO: -0.69661 factor:1 | 1 (-2.35613) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92938 HOMO: -6.76747 LUMO: -1.71976 factor:1 | 1 (-2.47264) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93414 HOMO: -6.48447 LUMO: -0.89525 factor:1 | 1 (-2.47741) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53280 HOMO: -7.11850 LUMO: -0.71566 factor:1 | 1 (-2.07607) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39371 HOMO: -6.80285 LUMO: -0.49253 factor:1 | 1 (-2.93698) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27393 HOMO: -6.80557 LUMO: -0.88165 factor:1 | 1 (-2.81719) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.81885 HOMO: -6.94162 LUMO: -0.08980 factor:1 | 1 (-1.36212) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80868 HOMO: -6.97972 LUMO: -0.29388 factor:1 | 1 (-1.35194) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74021 HOMO: -6.75114 LUMO: 0.04626 factor:1 | 1 (-1.28348) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69852 HOMO: -7.15932 LUMO: 0.68845 factor:1 | 1 (-2.24178) | 1 | 1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50809 HOMO: -7.36612 LUMO: 0.63675 factor:1 | 1 (-2.05136) | 1 | 1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79768 HOMO: -7.02598 LUMO: -0.66124 factor:1 | 1 (-1.34095) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.81499 HOMO: -6.89264 LUMO: -0.54967 factor:1 | 1 (-1.35826) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59473 HOMO: -6.97700 LUMO: 0.27756 factor:1 | 1 (-2.13800) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45378 HOMO: -6.60965 LUMO: 0.08163 factor:1 | 1 (-1.99704) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58011 HOMO: -6.70761 LUMO: 0.40001 factor:1 | 1 (-3.12338) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79966 HOMO: -6.69128 LUMO: 0.23674 factor:1 | 1 (-2.34293) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81185 HOMO: -6.69128 LUMO: -0.69933 factor:1 | 1 (-2.35512) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.70999 HOMO: -6.18515 LUMO: -0.85988 factor:1 | 1 (-3.25326) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.97770 HOMO: -6.86815 LUMO: -1.90208 factor:1 | 1 (-3.52096) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59060 HOMO: -6.37563 LUMO: -1.74697 factor:1 | 1 (-2.13386) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.97187 HOMO: -6.75659 LUMO: 0.36463 factor:1 | 1 (-3.51514) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.61695 HOMO: -6.91441 LUMO: -0.88981 factor:1 | 1 (-3.16022) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84665 HOMO: -6.71305 LUMO: -0.29933 factor:1 | 1 (-2.38992) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24233 HOMO: -6.91441 LUMO: -1.04492 factor:1 | 1 (-2.78560) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.28084 HOMO: -6.05453 LUMO: -0.83539 factor:1 | 1 (-2.82411) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20555 HOMO: -7.35252 LUMO: -0.45715 factor:1 | 1 (-2.74881) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65236 HOMO: -6.41644 LUMO: -0.97417 factor:1 | 1 (-2.19563) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.22304 HOMO: -6.78924 LUMO: 0.36735 factor:1 | 1 (-2.76631) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.98698 HOMO: -6.74298 LUMO: 0.51974 factor:1 | 1 (-2.53025) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11711 HOMO: -6.48992 LUMO: 1.44765 factor:1 | 1 (-2.66038) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.16505 HOMO: -6.12528 LUMO: 1.57826 factor:1 | 1 (-2.70832) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.71489 HOMO: -6.62325 LUMO: 1.57826 factor:1 | 1 (-3.25816) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.16415 HOMO: -6.19875 LUMO: 1.29798 factor:1 | 1 (-3.70742) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62066 HOMO: -6.74570 LUMO: 1.52112 factor:1 | 1 (-2.16393) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.17994 HOMO: -6.84094 LUMO: 1.48574 factor:1 | 1 (-2.72321) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24489 HOMO: -6.85183 LUMO: 0.33470 factor:1 | 1 (-2.78816) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13295 HOMO: -6.51168 LUMO: 0.48164 factor:1 | 1 (-2.67621) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24233 HOMO: -6.25046 LUMO: 0.75648 factor:1 | 1 (-2.78560) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.11865 HOMO: -6.65591 LUMO: 0.32109 factor:1 | 1 (-3.66192) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.84558 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-3.38885) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25357 HOMO: -6.75114 LUMO: 0.73471 factor:1 | 1 (-2.79684) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25643 HOMO: -6.50624 LUMO: 0.59321 factor:1 | 1 (-2.79970) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05486 HOMO: -6.39740 LUMO: 0.83267 factor:1 | 1 (-1.59812) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13817 HOMO: -6.44094 LUMO: 0.65579 factor:1 | 1 (-2.68144) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03760 HOMO: -6.52257 LUMO: 0.05714 factor:1 | 1 (-2.58086) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.48108 HOMO: -7.10217 LUMO: 0.49797 factor:1 | 1 (-4.02435) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.42903 HOMO: -6.83006 LUMO: 0.55783 factor:1 | 1 (-2.97230) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99322 HOMO: -6.99333 LUMO: -0.79457 factor:1 | 1 (-1.53649) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10179 HOMO: -6.64230 LUMO: 0.32382 factor:1 | 1 (-2.64506) | -1 | -1 |
| G: -6256.09104 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.97976 HOMO: -6.90897 LUMO: 0.30749 factor:1 | 1 (-3.52303) | -1 | -1 |
| G: -6256.09104 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20321 HOMO: -7.09129 LUMO: 1.33336 factor:1 | 1 (-2.74647) | 1 | 1 |
| G: -6256.09104 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07561 HOMO: -6.66951 LUMO: 1.34424 factor:1 | 1 (-2.61888) | -1 | -1 |
| G: -6256.09104 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.09479 HOMO: -7.02870 LUMO: 1.48574 factor:1 | 1 (-3.63805) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56091 HOMO: -7.26544 LUMO: 0.32926 factor:1 | 1 (-2.10417) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65808 HOMO: -6.56067 LUMO: -0.45987 factor:1 | 1 (-2.20135) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38912 HOMO: -6.54434 LUMO: -0.28300 factor:1 | 1 (-1.93239) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48639 HOMO: -7.19469 LUMO: 0.54695 factor:1 | 1 (-3.02966) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12356 HOMO: -6.47359 LUMO: -0.22041 factor:1 | 1 (-2.66682) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41271 HOMO: -6.80013 LUMO: 2.08167 factor:1 | 1 (-1.95598) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.59293 HOMO: -6.23957 LUMO: 1.67894 factor:1 | 1 (-3.13619) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08286 HOMO: -6.75114 LUMO: -0.62858 factor:1 | 1 (-1.62613) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.51328 HOMO: -6.79468 LUMO: -0.64491 factor:1 | 1 (-3.05655) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60080 HOMO: -6.84911 LUMO: -0.69661 factor:1 | 1 (-2.14407) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.87530 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-3.41857) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39687 HOMO: -6.92802 LUMO: -0.71022 factor:1 | 1 (-2.94014) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22257 HOMO: -6.72665 LUMO: -0.46804 factor:1 | 1 (-0.76584) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22681 HOMO: -6.63686 LUMO: -0.23674 factor:1 | 1 (-1.77007) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36899 HOMO: -7.21102 LUMO: 0.54423 factor:1 | 1 (-1.91225) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14923 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-1.69249) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08909 HOMO: -6.70761 LUMO: -0.31837 factor:1 | 1 (-1.63236) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23448 HOMO: -6.57155 LUMO: 1.76874 factor:1 | 1 (-1.77775) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62151 HOMO: -6.84366 LUMO: 2.04358 factor:1 | 1 (-2.16477) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26126 HOMO: -6.60420 LUMO: 1.80139 factor:1 | 1 (-1.80452) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.64109 HOMO: -7.03686 LUMO: 2.21229 factor:1 | 1 (-3.18436) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.09920 HOMO: -6.77564 LUMO: 1.97555 factor:1 | 1 (-2.64247) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65916 HOMO: -6.40012 LUMO: 2.17691 factor:1 | 1 (-3.20243) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94339 HOMO: -6.80013 LUMO: 2.25582 factor:1 | 1 (-2.48666) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15041 HOMO: -6.74298 LUMO: 2.31569 factor:1 | 1 (-2.69368) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33624 HOMO: -6.68856 LUMO: 1.85854 factor:1 | 1 (-2.87951) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.47502 HOMO: -6.17971 LUMO: 1.52928 factor:1 | 1 (-3.01829) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56104 HOMO: -6.54162 LUMO: 1.91840 factor:1 | 1 (-2.10431) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72020 HOMO: -6.80013 LUMO: -0.55511 factor:1 | 1 (-2.26347) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78156 HOMO: -7.46953 LUMO: 0.28572 factor:1 | 1 (-2.32483) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57699 HOMO: -6.61781 LUMO: -0.54967 factor:1 | 1 (-2.12026) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38839 HOMO: -6.56339 LUMO: -0.47892 factor:1 | 1 (-1.93165) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39329 HOMO: -6.65591 LUMO: -0.25307 factor:1 | 1 (-1.93655) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.82047 HOMO: -6.62869 LUMO: -0.23402 factor:1 | 1 (-3.36374) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47685 HOMO: -6.58243 LUMO: -0.19048 factor:1 | 1 (-2.02012) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13841 HOMO: -7.27632 LUMO: 0.52790 factor:1 | 1 (-2.68168) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.79826 HOMO: -7.21102 LUMO: 0.57688 factor:1 | 1 (-3.34153) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.98444 HOMO: -6.72393 LUMO: -0.53879 factor:1 | 1 (-3.52771) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.50607 HOMO: -7.42054 LUMO: -0.99322 factor:1 | 1 (-3.04934) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02494 HOMO: -6.88992 LUMO: -0.71838 factor:1 | 1 (-2.56821) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10429 HOMO: -6.88176 LUMO: -0.61226 factor:1 | 1 (-2.64756) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.16081 HOMO: -7.36340 LUMO: -1.04492 factor:1 | 1 (-2.70408) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27447 HOMO: -6.65863 LUMO: -0.41906 factor:1 | 1 (-2.81774) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30965 HOMO: -7.15115 LUMO: -0.66396 factor:1 | 1 (-0.85291) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.41328 HOMO: -7.10489 LUMO: -0.64491 factor:1 | 1 (-2.95654) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02000 HOMO: -7.20285 LUMO: 0.47892 factor:1 | 1 (-1.56327) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52716 HOMO: -6.55794 LUMO: -0.28844 factor:1 | 1 (-3.07042) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02902 HOMO: -7.19197 LUMO: -0.69661 factor:1 | 1 (-2.57229) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.54305 HOMO: -6.56883 LUMO: -0.32926 factor:1 | 1 (-0.08631) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91228 HOMO: -6.70761 LUMO: 1.95650 factor:1 | 1 (-0.45555) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68272 HOMO: -6.60420 LUMO: 1.80684 factor:1 | 1 (-3.22599) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79354 HOMO: -6.84094 LUMO: 1.64085 factor:1 | 1 (-2.33680) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31045 HOMO: -6.69128 LUMO: 1.90208 factor:1 | 1 (-1.85372) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36956 HOMO: -6.75387 LUMO: 1.70343 factor:1 | 1 (-1.91282) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38625 HOMO: -7.07496 LUMO: 2.10072 factor:1 | 1 (-0.92951) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29485 HOMO: -6.99877 LUMO: 2.24494 factor:1 | 1 (-2.83812) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.43872 HOMO: -6.63414 LUMO: 2.17691 factor:1 | 1 (-2.98199) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56243 HOMO: -6.44638 LUMO: 1.78235 factor:1 | 1 (-2.10570) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74015 HOMO: -6.87632 LUMO: 1.84221 factor:1 | 1 (-2.28342) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62464 HOMO: -6.85183 LUMO: 1.68711 factor:1 | 1 (-2.16790) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26097 HOMO: -6.96339 LUMO: 2.26671 factor:1 | 1 (-0.80423) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48463 HOMO: -6.63141 LUMO: 1.96738 factor:1 | 1 (-2.02790) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48039 HOMO: -6.37019 LUMO: 2.23133 factor:1 | 1 (-2.02366) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75873 HOMO: -7.11034 LUMO: 2.32385 factor:1 | 1 (-2.30200) | 1 | 1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23889 HOMO: -6.91986 LUMO: 1.65445 factor:1 | 1 (-1.78216) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.34235 HOMO: -7.12938 LUMO: 2.28304 factor:1 | 1 (-1.88561) | 1 | 1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04569 HOMO: -6.54978 LUMO: 1.92112 factor:1 | 1 (-1.58895) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.73374 HOMO: -6.83006 LUMO: 2.48712 factor:1 | 1 (-0.27701) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.25737 HOMO: -6.97972 LUMO: 1.96738 factor:1 | 1 (-0.80064) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45082 HOMO: -6.69944 LUMO: 2.06262 factor:1 | 1 (-0.99409) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.54029 HOMO: -6.76747 LUMO: 2.10888 factor:1 | 1 (-1.08356) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82952 HOMO: -6.91169 LUMO: 2.06534 factor:1 | 1 (-1.37279) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08544 HOMO: -7.03414 LUMO: 1.93473 factor:1 | 1 (-1.62871) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.04616 HOMO: -7.03142 LUMO: 2.52250 factor:1 | 1 (-0.58943) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20540 HOMO: -6.34025 LUMO: 2.61229 factor:1 | 1 (-0.74867) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24671 HOMO: -6.98788 LUMO: 2.28304 factor:1 | 1 (-0.78997) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23742 HOMO: -6.97700 LUMO: 2.53882 factor:1 | 1 (-1.78069) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.56269 HOMO: -6.58788 LUMO: 1.94289 factor:1 | 1 (-3.10596) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60192 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-2.14518) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.36313 HOMO: -6.55250 LUMO: 1.82861 factor:1 | -1 (0.09361) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43479 HOMO: -6.45998 LUMO: 1.75786 factor:1 | 1 (-0.97806) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.00142 HOMO: -6.78924 LUMO: 2.33746 factor:1 | 1 (-0.54469) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.66427 HOMO: -6.85727 LUMO: 1.76058 factor:1 | 1 (-1.20753) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.40231 HOMO: -6.70489 LUMO: 1.84493 factor:1 | 1 (-2.94558) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47922 HOMO: -6.71305 LUMO: 1.53472 factor:1 | 1 (-2.02249) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.50408 HOMO: -6.76747 LUMO: 1.48846 factor:1 | 1 (-3.04735) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71642 HOMO: -6.69128 LUMO: 1.95922 factor:1 | 1 (-2.25969) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.66023 HOMO: -6.67495 LUMO: 2.05446 factor:1 | 1 (-2.20350) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.37511 HOMO: -6.63686 LUMO: 2.25310 factor:1 | 1 (-1.91838) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47870 HOMO: -6.63958 LUMO: 2.14154 factor:1 | 1 (-2.02197) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.43870 HOMO: -6.62597 LUMO: 2.01908 factor:1 | 1 (-1.98197) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.25854 HOMO: -7.07768 LUMO: 2.14154 factor:1 | 1 (-0.80181) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50145 HOMO: -6.19603 LUMO: 2.01092 factor:1 | 1 (-2.04472) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.18235 HOMO: -6.65046 LUMO: 2.15786 factor:1 | 1 (-0.72562) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70423 HOMO: -6.92258 LUMO: 2.31841 factor:1 | 1 (-2.24750) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.20158 HOMO: -6.90081 LUMO: 2.19324 factor:1 | 1 (-1.74485) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.03454 HOMO: -6.85455 LUMO: 1.95650 factor:1 | 1 (-0.57781) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13179 HOMO: -6.57699 LUMO: 1.76058 factor:1 | 1 (-0.67506) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84185 HOMO: -6.90625 LUMO: 1.97555 factor:1 | 1 (-1.38511) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21133 HOMO: -6.97428 LUMO: 1.92929 factor:1 | 1 (-0.75460) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.31531 HOMO: -6.61781 LUMO: -0.41906 factor:1 | 1 (-3.85857) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.00643 HOMO: -6.62869 LUMO: -0.81906 factor:1 | 1 (-3.54970) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29757 HOMO: -7.01237 LUMO: 2.00548 factor:1 | 1 (-2.84084) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.14532 HOMO: -6.85727 LUMO: 2.17691 factor:1 | 1 (-3.68859) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.90825 HOMO: -6.71849 LUMO: 1.58914 factor:1 | 1 (-3.45152) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30064 HOMO: -7.52395 LUMO: 0.27211 factor:1 | 1 (-0.84391) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08240 HOMO: -6.96611 LUMO: -0.72654 factor:1 | 1 (-1.62566) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17622 HOMO: -6.89537 LUMO: -0.68028 factor:1 | 1 (-1.71949) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03513 HOMO: -6.84911 LUMO: -0.58504 factor:1 | 1 (-1.57840) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.85231 HOMO: -6.79196 LUMO: -0.55783 factor:1 | 1 (-3.39557) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.02009 HOMO: -6.67767 LUMO: 1.79323 factor:1 | 1 (-3.56336) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12236 HOMO: -6.54434 LUMO: 1.91024 factor:1 | 1 (-2.66563) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20231 HOMO: -6.62869 LUMO: 1.69799 factor:1 | 1 (-2.74557) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.28105 HOMO: -6.72393 LUMO: 2.12249 factor:1 | 1 (-3.82432) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.67486 HOMO: -6.66407 LUMO: 2.05990 factor:1 | 1 (-3.21813) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.08282 HOMO: -7.00149 LUMO: 1.82044 factor:1 | 1 (-2.62609) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38213 HOMO: -7.12122 LUMO: 2.16058 factor:1 | 1 (-1.92540) | 1 | 1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.17253 HOMO: -6.63141 LUMO: 2.21229 factor:1 | 1 (-3.71580) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.40182 HOMO: -6.37835 LUMO: 2.32113 factor:1 | 1 (-2.94509) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92546 HOMO: -6.99605 LUMO: 2.00548 factor:1 | 1 (-2.46873) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15452 HOMO: -6.85999 LUMO: 2.39460 factor:1 | 1 (-2.69779) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32553 HOMO: -6.85727 LUMO: 2.48712 factor:1 | 1 (-1.86880) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.53766 HOMO: -7.04231 LUMO: 2.40277 factor:1 | 1 (-3.08093) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18438 HOMO: -6.60692 LUMO: 2.26671 factor:1 | 1 (-1.72765) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.16040 HOMO: -6.67495 LUMO: 2.14698 factor:1 | 1 (-2.70367) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.40005 HOMO: -6.73210 LUMO: 2.06807 factor:1 | 1 (-2.94332) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55070 HOMO: -7.20013 LUMO: 2.02181 factor:1 | 1 (-2.09397) | 1 | 1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.77829 HOMO: -7.18653 LUMO: 2.29936 factor:1 | 1 (-3.32156) | 1 | 1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93286 HOMO: -6.92802 LUMO: 2.36195 factor:1 | 1 (-2.47613) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30070 HOMO: -6.89537 LUMO: 1.78779 factor:1 | 1 (-2.84397) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.31005 HOMO: -6.96067 LUMO: 2.31297 factor:1 | 1 (-0.85332) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26711 HOMO: -6.91441 LUMO: 2.50345 factor:1 | 1 (-0.81038) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29242 HOMO: -7.17292 LUMO: 2.12521 factor:1 | 1 (-0.83569) | 1 | 1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20790 HOMO: -6.93618 LUMO: 2.35106 factor:1 | 1 (-0.75117) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24287 HOMO: -6.75931 LUMO: 1.61908 factor:1 | 1 (-0.78614) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.06706 HOMO: -6.35930 LUMO: 1.23540 factor:1 | 1 (-0.61032) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65471 HOMO: -6.17971 LUMO: 1.84493 factor:1 | 1 (-2.19797) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70173 HOMO: -6.72665 LUMO: 2.61229 factor:1 | 1 (-2.24499) | -1 | -1 |
| G: -6256.09104 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56679 HOMO: -6.62869 LUMO: 2.28304 factor:1 | 1 (-2.11005) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42578 HOMO: -6.58243 LUMO: 0.28028 factor:1 | 1 (-1.96904) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15988 HOMO: -6.79468 LUMO: 0.14966 factor:1 | 1 (-2.70315) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.09997 HOMO: -6.63141 LUMO: 0.31021 factor:1 | 1 (-2.64323) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48609 HOMO: -6.81101 LUMO: 0.13878 factor:1 | 1 (-3.02936) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.53956 HOMO: -6.72665 LUMO: 0.65579 factor:1 | 1 (-3.08283) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06223 HOMO: -6.53073 LUMO: 0.91430 factor:1 | 1 (-1.60550) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13649 HOMO: -7.19197 LUMO: 1.62996 factor:1 | 1 (-1.67976) | 1 | 1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33712 HOMO: -6.69400 LUMO: 0.84627 factor:1 | 1 (-1.88039) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24923 HOMO: -6.76475 LUMO: 0.51974 factor:1 | 1 (-1.79250) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28477 HOMO: -6.67767 LUMO: 0.52246 factor:1 | 1 (-1.82803) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41388 HOMO: -6.73210 LUMO: 0.94424 factor:1 | 1 (-1.95715) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46442 HOMO: -6.97972 LUMO: 0.60409 factor:1 | 1 (-2.00768) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13486 HOMO: -7.38517 LUMO: 0.73743 factor:1 | 1 (-1.67813) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40681 HOMO: -6.48992 LUMO: 1.08301 factor:1 | 1 (-1.95008) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14359 HOMO: -7.18381 LUMO: 1.61908 factor:1 | 1 (-1.68686) | 1 | 1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46768 HOMO: -6.74842 LUMO: 0.57960 factor:1 | 1 (-2.01095) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03954 HOMO: -6.67495 LUMO: 0.77280 factor:1 | 1 (-1.58280) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25200 HOMO: -6.74570 LUMO: 0.77280 factor:1 | 1 (-1.79527) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46178 HOMO: -6.73754 LUMO: 0.86804 factor:1 | 1 (-2.00504) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23777 HOMO: -6.66135 LUMO: 0.94424 factor:1 | 1 (-1.78104) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.49525 HOMO: -6.44638 LUMO: 1.00138 factor:1 | 1 (-2.03851) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.34406 HOMO: -6.65591 LUMO: 1.02043 factor:1 | 1 (-1.88733) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18727 HOMO: -7.17564 LUMO: 0.50069 factor:1 | 1 (-1.73054) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28207 HOMO: -6.59332 LUMO: 0.79457 factor:1 | 1 (-1.82534) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24686 HOMO: -6.76747 LUMO: 1.73881 factor:1 | 1 (-1.79013) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47070 HOMO: -7.00421 LUMO: 1.07485 factor:1 | 1 (-2.01397) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79128 HOMO: -6.94979 LUMO: 1.67894 factor:1 | 1 (-2.33455) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90350 HOMO: -6.66135 LUMO: 0.47076 factor:1 | 1 (-2.44677) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99939 HOMO: -6.74298 LUMO: 1.85037 factor:1 | 1 (-2.54266) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81604 HOMO: -6.65318 LUMO: 0.95240 factor:1 | 1 (-2.35931) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.87456 HOMO: -6.63958 LUMO: 0.78097 factor:1 | 1 (-3.41783) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.40500 HOMO: -6.11712 LUMO: 0.40001 factor:1 | 1 (-3.94826) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54521 HOMO: -7.08312 LUMO: 0.92519 factor:1 | 1 (-2.08847) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14380 HOMO: -6.96067 LUMO: 0.54695 factor:1 | 1 (-2.68707) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.17959 HOMO: -6.74026 LUMO: 0.60137 factor:1 | 1 (-2.72285) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93278 HOMO: -6.74298 LUMO: 0.59593 factor:1 | 1 (-2.47605) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35383 HOMO: -6.93074 LUMO: 0.60681 factor:1 | 1 (-1.89710) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32243 HOMO: -6.41644 LUMO: 0.35919 factor:1 | 1 (-1.86569) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53280 HOMO: -6.41917 LUMO: 1.73064 factor:1 | 1 (-2.07607) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.05756 HOMO: -4.64226 LUMO: -0.87893 factor:1 | 1 (-0.60083) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88541 HOMO: -6.59604 LUMO: 0.90342 factor:1 | 1 (-1.42868) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32635 HOMO: -6.79468 LUMO: 0.50069 factor:1 | 1 (-1.86961) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24403 HOMO: -7.04503 LUMO: 0.52518 factor:1 | 1 (-1.78730) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87997 HOMO: -6.69400 LUMO: 0.54423 factor:1 | 1 (-1.42324) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28175 HOMO: -6.51713 LUMO: 0.95240 factor:1 | 1 (-1.82501) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11674 HOMO: -6.88176 LUMO: 1.79323 factor:1 | 1 (-1.66000) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.04018 HOMO: -6.71849 LUMO: 0.28844 factor:1 | 1 (-2.58345) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.16127 HOMO: -6.94979 LUMO: 0.51974 factor:1 | 1 (-2.70454) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.72077 HOMO: -6.76203 LUMO: 0.94151 factor:1 | 1 (-3.26403) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81819 HOMO: -6.91169 LUMO: 0.89525 factor:1 | 1 (-2.36146) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.82965 HOMO: -6.83006 LUMO: 0.89253 factor:1 | 1 (-2.37291) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30278 HOMO: -7.08857 LUMO: 0.60409 factor:1 | 1 (-1.84605) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24343 HOMO: -6.91713 LUMO: 1.76330 factor:1 | 1 (-1.78670) | -1 | -1 |
| G: -6256.09104 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78306 HOMO: -6.47359 LUMO: 1.56193 factor:1 | 1 (-2.32633) | -1 | -1 |
| G: -6256.09104 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.86010 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-2.40336) | -1 | -1 |
| G: -6256.09104 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23312 HOMO: -7.03686 LUMO: 1.97283 factor:1 | 1 (-1.77639) | -1 | -1 |
| G: -6256.09104 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14795 HOMO: -7.00965 LUMO: 1.64629 factor:1 | 1 (-1.69121) | -1 | -1 |
| G: -6256.09104 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.77231 HOMO: -7.06952 LUMO: 1.67622 factor:1 | 1 (-2.31558) | 1 | -1 |
| G: -6256.09104 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.66224 HOMO: -6.80557 LUMO: 1.70615 factor:1 | 1 (-2.20551) | -1 | -1 |
| G: -6256.09104 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18928 HOMO: -6.80829 LUMO: 1.71704 factor:1 | 1 (-1.73255) | -1 | -1 |
| G: -6256.09104 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98846 HOMO: -7.26544 LUMO: 1.89935 factor:1 | 1 (-1.53173) | 1 | -1 |
| G: -6256.09104 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.41554 HOMO: -7.00149 LUMO: 1.47214 factor:1 | 1 (-2.95880) | -1 | -1 |
| G: -6256.09104 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.12137 HOMO: -7.03686 LUMO: 1.97283 factor:1 | 1 (-3.66464) | -1 | -1 |
| G: -6256.09104 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.18145 HOMO: -7.00965 LUMO: 1.64629 factor:1 | 1 (-3.72472) | -1 | -1 |
| G: -6256.09104 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71144 HOMO: -7.06952 LUMO: 1.67622 factor:1 | 1 (-2.25471) | -1 | -1 |
| G: -6256.09104 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17608 HOMO: -6.80557 LUMO: 1.70615 factor:1 | 1 (-1.71935) | -1 | -1 |
| G: -6256.09104 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58991 HOMO: -6.80829 LUMO: 1.71704 factor:1 | 1 (-3.13317) | -1 | -1 |
| G: -6256.09104 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.07348 HOMO: -7.26544 LUMO: 1.89935 factor:1 | 1 (-3.61675) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12386 HOMO: -7.00149 LUMO: 1.75241 factor:1 | 1 (-2.66712) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86419 HOMO: -6.91169 LUMO: 2.07079 factor:1 | 1 (-1.40745) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18444 HOMO: -7.11034 LUMO: 1.76330 factor:1 | 1 (-1.72771) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92998 HOMO: -6.87360 LUMO: 2.02725 factor:1 | 1 (-1.47325) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.53592 HOMO: -7.08584 LUMO: 1.82044 factor:1 | 1 (-3.07919) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.93919 HOMO: -6.90625 LUMO: 1.68166 factor:1 | 1 (-3.48246) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12407 HOMO: -6.71577 LUMO: 1.93201 factor:1 | 1 (-2.66734) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62643 HOMO: -6.99605 LUMO: 2.08439 factor:1 | 1 (-2.16970) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82791 HOMO: -7.02326 LUMO: 1.97010 factor:1 | 1 (-1.37118) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06577 HOMO: -6.99877 LUMO: 2.15514 factor:1 | 1 (-1.60904) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62962 HOMO: -6.75387 LUMO: 1.95106 factor:1 | 1 (-2.17288) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88644 HOMO: -7.10761 LUMO: 2.06262 factor:1 | 1 (-2.42970) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.72240 HOMO: -7.03142 LUMO: 1.91568 factor:1 | 1 (-3.26567) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58506 HOMO: -6.98788 LUMO: 1.98371 factor:1 | 1 (-3.12833) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10503 HOMO: -6.94707 LUMO: 1.68438 factor:1 | 1 (-2.64829) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.55483 HOMO: -6.88176 LUMO: 2.20684 factor:1 | 1 (-3.09810) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.85531 HOMO: -6.73210 LUMO: 2.18780 factor:1 | 1 (-2.39857) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88217 HOMO: -6.83822 LUMO: 2.06807 factor:1 | 1 (-2.42543) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18350 HOMO: -6.78924 LUMO: 2.42181 factor:1 | 1 (-2.72677) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32498 HOMO: -6.94707 LUMO: 1.71704 factor:1 | 1 (-1.86825) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28673 HOMO: -6.85183 LUMO: 1.78779 factor:1 | 1 (-0.83000) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52709 HOMO: -6.98788 LUMO: 1.69799 factor:1 | 1 (-1.07036) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.63118 HOMO: -6.79468 LUMO: 2.04358 factor:1 | 1 (-0.17445) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89485 HOMO: -6.90081 LUMO: 1.97283 factor:1 | 1 (-1.43812) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78612 HOMO: -6.79468 LUMO: 2.00820 factor:1 | 1 (-1.32939) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24695 HOMO: -7.06408 LUMO: 2.29936 factor:1 | 1 (-0.79022) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45307 HOMO: -6.78924 LUMO: 2.13337 factor:1 | 1 (-1.99634) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65634 HOMO: -6.79468 LUMO: 2.35106 factor:1 | 1 (-2.19961) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08278 HOMO: -6.82734 LUMO: 2.16603 factor:1 | 1 (-1.62604) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96465 HOMO: -6.79740 LUMO: 2.36739 factor:1 | 1 (-1.50792) | -1 | -1 |
| G: -6256.09104 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97159 HOMO: -7.14027 LUMO: 2.10888 factor:1 | 1 (-1.51486) | -1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95023 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.49350) | -1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.59009 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.13335) | -1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.69554 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-3.23881) | -1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87419 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-2.41746) | -1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80918 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-2.35245) | -1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71264 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-2.25591) | -1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03058 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-2.57384) | -1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43988 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-0.98315) | -1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73931 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-2.28257) | -1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48597 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-2.02923) | -1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98628 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-1.52955) | -1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89610 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-2.43936) | -1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74633 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-2.28959) | -1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99940 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.54267) | 1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57248 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.11575) | 1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.56516 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.10843) | -1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76350 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-2.30676) | 1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67699 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-2.22026) | -1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22275 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.76602) | 1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65946 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-3.20273) | -1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.04738 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-3.59065) | -1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.16342 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-2.70669) | -1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.90148 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-3.44474) | -1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.00176 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-2.54503) | -1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.17567 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-2.71893) | -1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91833 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-2.46160) | -1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42191 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-1.96518) | -1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70951 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-2.25278) | -1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46575 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-2.00902) | -1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39972 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.94298) | -1 | -1 |
| G: -6256.09104 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33942 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.88268) | 1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94108 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-2.48435) | -1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06747 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-2.61074) | -1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.29334 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.83661) | -1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11418 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-1.65745) | -1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.87190 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-3.41517) | -1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.25231 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-3.79558) | -1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.74561 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-3.28888) | -1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.04194 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-3.58521) | -1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.94232 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-3.48559) | -1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23186 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-2.77513) | -1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06327 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-1.60653) | -1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88548 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-2.42875) | -1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90157 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-2.44483) | -1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.85052 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-2.39379) | 1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16980 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.71307) | 1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.73492 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-3.27818) | -1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.66286 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-3.20613) | 1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10824 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-2.65150) | -1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.86836 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-3.41163) | 1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13763 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-2.68089) | -1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14179 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-2.68506) | -1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.27560 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.81887) | -1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.27626 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.81953) | -1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95837 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-1.50163) | -1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04563 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-1.58890) | -1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92528 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.46854) | -1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04637 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-1.58963) | -1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12026 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-0.66352) | -1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91057 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-2.45384) | -1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.04592 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-2.58919) | -1 | -1 |
| G: -6256.09104 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.80289 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-3.34616) | 1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33151 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-2.87477) | -1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96486 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-2.50813) | -1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19051 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-0.73378) | -1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.05797 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.60124) | -1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88272 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.42599) | -1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83033 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-2.37359) | -1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59762 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-2.14088) | -1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14974 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.69301) | -1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91085 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-2.45411) | -1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86704 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-1.41031) | -1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00095 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-1.54422) | -1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83235 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.37562) | -1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68967 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-2.23294) | -1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95056 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.49382) | -1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69740 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-2.24067) | -1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97839 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.52166) | -1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94206 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-2.48532) | -1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72603 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-2.26929) | -1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84323 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-2.38649) | -1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93961 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-2.48288) | -1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02211 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-2.56538) | -1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07052 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-2.61379) | -1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15114 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.69441) | -1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07850 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-1.62177) | -1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98552 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-1.52879) | -1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84100 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.38427) | -1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58737 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-1.13063) | -1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06767 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-1.61094) | -1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05739 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.60066) | -1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04582 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-1.58909) | -1 | -1 |
| G: -6256.09104 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92707 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.47034) | -1 | -1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90917 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.45243) | 1 | 1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.71572 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-1.25899) | -1 | -1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91744 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.46071) | 1 | 1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83841 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-2.38168) | -1 | -1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76769 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-2.31095) | -1 | -1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84233 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-2.38560) | 1 | 1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54853 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-2.09179) | 1 | 1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87030 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-2.41357) | 1 | 1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74722 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-2.29049) | 1 | 1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68635 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-2.22962) | 1 | 1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80924 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-2.35251) | 1 | 1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19154 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.73481) | 1 | 1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32379 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.86705) | -1 | -1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03741 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.58068) | -1 | -1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01880 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.56207) | -1 | -1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06411 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.60738) | 1 | 1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99815 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.54142) | 1 | 1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97001 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-1.51328) | 1 | 1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72480 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-2.26807) | 1 | 1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65484 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-2.19811) | 1 | 1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96954 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-2.51281) | 1 | 1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55555 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-2.09881) | 1 | 1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68989 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-2.23316) | 1 | 1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80943 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-2.35270) | 1 | 1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.98316 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-3.52643) | 1 | 1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30895 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-2.85222) | 1 | 1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52269 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-3.06596) | 1 | 1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.98814 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-3.53141) | 1 | 1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.82132 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-2.36459) | -1 | -1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.43718 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-1.98044) | 1 | 1 |
| G: -6256.09104 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57933 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-2.12260) | 1 | 1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67517 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-2.21844) | 1 | 1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16823 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.71150) | -1 | -1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15963 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-0.70290) | 1 | 1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74018 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-2.28344) | -1 | -1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.66499 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-2.20826) | -1 | -1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88521 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-2.42848) | -1 | -1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38080 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-1.92406) | 1 | 1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33070 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.87397) | 1 | 1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35263 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-1.89590) | 1 | 1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78962 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-2.33289) | 1 | 1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.18573 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.72899) | 1 | 1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21196 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-0.75522) | 1 | 1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37697 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-0.92023) | -1 | -1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11138 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.65464) | -1 | -1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76690 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-2.31017) | -1 | -1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30251 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.84578) | 1 | 1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30178 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.84505) | 1 | 1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30872 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.85199) | 1 | 1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26336 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.80663) | 1 | 1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.11650 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-0.65977) | 1 | 1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.17032 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-0.71359) | 1 | 1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33808 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.88135) | 1 | 1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88060 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-1.42386) | 1 | 1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86212 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-1.40539) | 1 | 1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79700 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-1.34027) | 1 | 1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37876 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-0.92203) | 1 | 1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16809 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.71136) | 1 | 1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09038 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-0.63364) | 1 | 1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.00556 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.54883) | -1 | -1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45647 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-1.99974) | 1 | 1 |
| G: -6256.09104 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10231 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-2.64557) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.06923 HOMO: -7.06135 LUMO: 0.75376 factor:1 | 1 (-0.61250) | 1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.89309 HOMO: -5.10213 LUMO: 0.77825 factor:1 | 1 (-0.43636) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.66028 HOMO: -5.84228 LUMO: 0.50341 factor:1 | 1 (-2.20355) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84772 HOMO: -5.39874 LUMO: 0.68028 factor:1 | 1 (-1.39099) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05937 HOMO: -5.16744 LUMO: 1.14832 factor:1 | 1 (-1.60264) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.68519 HOMO: -5.80963 LUMO: 0.35647 factor:1 | 1 (-1.22846) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78027 HOMO: -5.02322 LUMO: 1.07213 factor:1 | 1 (-1.32353) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45406 HOMO: -5.80963 LUMO: 0.56328 factor:1 | 1 (-0.99732) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38997 HOMO: -5.45316 LUMO: 0.78369 factor:1 | 1 (-0.93324) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.49702 HOMO: -5.25452 LUMO: 0.82178 factor:1 | 1 (-1.04029) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43969 HOMO: -5.21370 LUMO: 1.03947 factor:1 | 1 (-0.98296) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.50214 HOMO: -6.04365 LUMO: 0.31837 factor:1 | 1 (-1.04541) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.59226 HOMO: -5.86405 LUMO: 0.55511 factor:1 | 1 (-1.13553) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53915 HOMO: -5.64908 LUMO: 0.71022 factor:1 | 1 (-1.08241) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53945 HOMO: -5.94297 LUMO: 0.68301 factor:1 | 1 (-1.08271) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.63368 HOMO: -6.01916 LUMO: 0.56328 factor:1 | 1 (-1.17695) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62763 HOMO: -6.05181 LUMO: 0.35103 factor:1 | 1 (-2.17090) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70271 HOMO: -6.08447 LUMO: 0.48436 factor:1 | 1 (-2.24597) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73218 HOMO: -5.86950 LUMO: 0.36735 factor:1 | 1 (-2.27544) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54053 HOMO: -5.33615 LUMO: 0.65852 factor:1 | 1 (-2.08379) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14370 HOMO: -5.36064 LUMO: 0.86804 factor:1 | 1 (-1.68697) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22569 HOMO: -5.74160 LUMO: 0.64491 factor:1 | 1 (-1.76896) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12071 HOMO: -5.23003 LUMO: 0.66124 factor:1 | 1 (-1.66398) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20355 HOMO: -5.77698 LUMO: 0.84083 factor:1 | 1 (-0.74682) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44379 HOMO: -5.60555 LUMO: 0.84355 factor:1 | 1 (-1.98706) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60115 HOMO: -7.11578 LUMO: -1.62452 factor:1 | 1 (-2.14442) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71193 HOMO: -7.23279 LUMO: -1.63813 factor:1 | 1 (-2.25520) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22368 HOMO: -6.68312 LUMO: -0.88709 factor:1 | 1 (-1.76694) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78448 HOMO: -6.99333 LUMO: -0.88709 factor:1 | 1 (-2.32774) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44453 HOMO: -7.40694 LUMO: 0.11973 factor:1 | 1 (-0.98780) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.49335 HOMO: -6.74026 LUMO: -0.72927 factor:1 | 1 (-1.03662) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39999 HOMO: -6.67223 LUMO: -0.70750 factor:1 | 1 (-0.94326) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.42894 HOMO: -7.06952 LUMO: -1.40139 factor:1 | 1 (-0.97221) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.40864 HOMO: -7.21374 LUMO: -1.13199 factor:1 | 1 (-0.95191) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19370 HOMO: -6.54706 LUMO: -1.34424 factor:1 | 1 (-0.73697) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12243 HOMO: -7.51851 LUMO: -1.05852 factor:1 | 1 (-0.66570) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.08643 HOMO: -7.07224 LUMO: -1.89391 factor:1 | 1 (-0.62970) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96786 HOMO: -6.65863 LUMO: -0.46804 factor:1 | 1 (-1.51113) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06433 HOMO: -7.24367 LUMO: 0.29388 factor:1 | 1 (-1.60759) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.54873 HOMO: -7.02326 LUMO: -0.87893 factor:1 | 1 (-1.09199) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.75621 HOMO: -6.88176 LUMO: 0.71566 factor:1 | 1 (-1.29948) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00822 HOMO: -6.46543 LUMO: 1.01498 factor:1 | 1 (-1.55148) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02735 HOMO: -6.30760 LUMO: 0.17687 factor:1 | 1 (-1.57061) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00718 HOMO: -6.73210 LUMO: -1.06941 factor:1 | 1 (-1.55045) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00778 HOMO: -6.83550 LUMO: -0.75920 factor:1 | 1 (-1.55105) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05935 HOMO: -6.94707 LUMO: 0.42178 factor:1 | 1 (-1.60261) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.49779 HOMO: -6.77019 LUMO: -0.38096 factor:1 | 1 (-1.04105) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.76473 HOMO: -7.34163 LUMO: 0.35103 factor:1 | 1 (-1.30800) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.49057 HOMO: -6.87632 LUMO: -0.87349 factor:1 | 1 (-1.03384) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43202 HOMO: -7.06952 LUMO: -1.47214 factor:1 | 1 (-0.97528) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43768 HOMO: -6.58788 LUMO: -0.37824 factor:1 | 1 (-0.98094) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.06463 HOMO: -6.92802 LUMO: -1.24900 factor:1 | 1 (-0.60790) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.81481 HOMO: -7.01237 LUMO: -1.31975 factor:1 | 1 (-0.35807) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.80771 HOMO: -6.74842 LUMO: 0.45987 factor:1 | 1 (-0.35097) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96950 HOMO: -6.53890 LUMO: 0.94424 factor:1 | 1 (-1.51276) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08335 HOMO: -6.52257 LUMO: -0.66940 factor:1 | 1 (-1.62662) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17535 HOMO: -6.56883 LUMO: -1.48302 factor:1 | 1 (-1.71862) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33207 HOMO: -7.21646 LUMO: 0.13061 factor:1 | 1 (-0.87534) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.49011 HOMO: -6.62597 LUMO: -0.64763 factor:1 | 1 (-1.03338) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.51175 HOMO: -7.38789 LUMO: 0.31021 factor:1 | 1 (-1.05501) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99322 HOMO: -6.74570 LUMO: -0.70750 factor:1 | 1 (-1.53649) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28586 HOMO: -6.95251 LUMO: -1.25989 factor:1 | 1 (-0.82913) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58554 HOMO: -7.13483 LUMO: -0.76736 factor:1 | 1 (-1.12881) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01799 HOMO: -6.93618 LUMO: -1.24628 factor:1 | 1 (-1.56125) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07127 HOMO: -7.03686 LUMO: 0.26395 factor:1 | 1 (-1.61453) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14563 HOMO: -6.52257 LUMO: -0.84355 factor:1 | 1 (-1.68890) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05556 HOMO: -6.83278 LUMO: -0.49525 factor:1 | 1 (-1.59883) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30395 HOMO: -7.18381 LUMO: -1.64629 factor:1 | 1 (-1.84722) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.62168 HOMO: -6.74842 LUMO: -0.81090 factor:1 | 1 (-1.16495) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96003 HOMO: -7.09401 LUMO: -0.92519 factor:1 | 1 (-1.50329) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01061 HOMO: -7.20285 LUMO: -0.81634 factor:1 | 1 (-1.55388) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08098 HOMO: -6.72665 LUMO: 0.77008 factor:1 | 1 (-1.62425) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.21965 HOMO: -6.80829 LUMO: 0.86532 factor:1 | 1 (-1.76292) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85698 HOMO: -6.20964 LUMO: 0.99866 factor:1 | 1 (-1.40024) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10721 HOMO: -6.52801 LUMO: 1.07757 factor:1 | 1 (-1.65048) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92321 HOMO: -6.74298 LUMO: -0.67756 factor:1 | 1 (-1.46648) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05524 HOMO: -7.43959 LUMO: 0.03265 factor:1 | 1 (-1.59851) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15789 HOMO: -6.46815 LUMO: -0.29933 factor:1 | 1 (-0.70116) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.94518 HOMO: -6.70489 LUMO: -0.97145 factor:1 | 1 (-0.48844) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04824 HOMO: -6.30216 LUMO: -1.39322 factor:1 | 1 (-1.59151) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02740 HOMO: -7.01782 LUMO: -1.07485 factor:1 | 1 (-1.57067) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04672 HOMO: -6.93074 LUMO: 0.25851 factor:1 | 1 (-1.58999) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00337 HOMO: -7.07224 LUMO: 0.09524 factor:1 | 1 (-1.54664) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03094 HOMO: -6.62325 LUMO: -0.45443 factor:1 | 1 (-1.57421) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03967 HOMO: -7.09945 LUMO: -1.20274 factor:1 | 1 (-1.58294) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.73039 HOMO: -6.56067 LUMO: -1.39322 factor:1 | 1 (-1.27366) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.66603 HOMO: -6.75387 LUMO: -0.72654 factor:1 | 1 (-1.20930) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77752 HOMO: -6.28583 LUMO: -2.35651 factor:1 | 1 (-1.32079) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85831 HOMO: -6.55522 LUMO: -1.33608 factor:1 | 1 (-1.40158) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91202 HOMO: -7.19741 LUMO: -0.93607 factor:1 | 1 (-1.45529) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.72941 HOMO: -6.39740 LUMO: -1.14832 factor:1 | 1 (-1.27268) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08182 HOMO: -7.11850 LUMO: -0.97417 factor:1 | 1 (-1.62509) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89028 HOMO: -6.57699 LUMO: -1.14016 factor:1 | 1 (-1.43355) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22928 HOMO: -6.57699 LUMO: -1.31975 factor:1 | 1 (-1.77255) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52930 HOMO: -6.69128 LUMO: -0.76736 factor:1 | 1 (-1.07256) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82827 HOMO: -7.25728 LUMO: 0.29660 factor:1 | 1 (-1.37154) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12403 HOMO: -6.37019 LUMO: -0.95240 factor:1 | 1 (-1.66730) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.61003 HOMO: -6.48447 LUMO: -0.55511 factor:1 | 1 (-1.15330) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58375 HOMO: -6.37291 LUMO: -0.78641 factor:1 | 1 (-1.12701) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12642 HOMO: -6.65863 LUMO: -0.69933 factor:1 | 1 (-1.66969) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35562 HOMO: -6.44638 LUMO: -0.16055 factor:1 | 1 (-1.89889) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23274 HOMO: -6.41917 LUMO: -0.20136 factor:1 | 1 (-1.77601) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.21165 HOMO: -7.33347 LUMO: 0.12789 factor:1 | 1 (-1.75492) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88163 HOMO: -6.70489 LUMO: -0.52518 factor:1 | 1 (-1.42490) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00672 HOMO: -7.25183 LUMO: 0.32109 factor:1 | 1 (-1.54999) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79153 HOMO: -7.29265 LUMO: 0.28028 factor:1 | 1 (-1.33480) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84508 HOMO: -6.57155 LUMO: -0.51702 factor:1 | 1 (-1.38835) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09393 HOMO: -7.08040 LUMO: 0.39729 factor:1 | 1 (-1.63720) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19750 HOMO: -6.24501 LUMO: -0.44627 factor:1 | 1 (-1.74077) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58807 HOMO: -6.73754 LUMO: -0.45443 factor:1 | 1 (-1.13134) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09336 HOMO: -6.24501 LUMO: 0.38096 factor:1 | 1 (-1.63663) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.68761 HOMO: -6.86815 LUMO: -0.91974 factor:1 | 1 (-1.23088) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79880 HOMO: -7.40150 LUMO: 0.36191 factor:1 | 1 (-1.34207) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79542 HOMO: -6.44094 LUMO: -0.64219 factor:1 | 1 (-1.33869) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.73110 HOMO: -6.69944 LUMO: -0.80001 factor:1 | 1 (-1.27436) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05137 HOMO: -6.61509 LUMO: -0.70750 factor:1 | 1 (-1.59464) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47876 HOMO: -7.52123 LUMO: 0.06803 factor:1 | 1 (-2.02202) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69294 HOMO: -7.34163 LUMO: 0.30477 factor:1 | 1 (-2.23620) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84535 HOMO: -6.68584 LUMO: -0.78641 factor:1 | 1 (-2.38862) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58589 HOMO: -6.53890 LUMO: -0.50885 factor:1 | 1 (-2.12915) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60540 HOMO: -6.75659 LUMO: -0.68845 factor:1 | 1 (-2.14867) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.62266 HOMO: -7.08857 LUMO: 0.43266 factor:1 | 1 (-1.16593) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.63870 HOMO: -6.28583 LUMO: -0.46804 factor:1 | 1 (-2.18197) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59772 HOMO: -6.50080 LUMO: -0.24762 factor:1 | 1 (-2.14099) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55383 HOMO: -6.45454 LUMO: -0.58504 factor:1 | 1 (-2.09710) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79552 HOMO: -7.20558 LUMO: 0.20953 factor:1 | 1 (-2.33879) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.40649 HOMO: -6.35930 LUMO: -0.20681 factor:1 | 1 (-0.94976) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.47501 HOMO: -6.36202 LUMO: -0.14422 factor:1 | 1 (-1.01828) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98737 HOMO: -6.20692 LUMO: 1.97827 factor:1 | 1 (-1.53064) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86498 HOMO: -6.48719 LUMO: 1.74153 factor:1 | 1 (-1.40824) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94389 HOMO: -6.84638 LUMO: 1.88575 factor:1 | 1 (-1.48716) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.62715 HOMO: -5.90759 LUMO: 2.00820 factor:1 | 1 (-1.17042) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85216 HOMO: -6.56339 LUMO: 1.99732 factor:1 | 1 (-1.39543) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83869 HOMO: -6.20692 LUMO: 1.75241 factor:1 | 1 (-1.38196) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93611 HOMO: -6.16882 LUMO: 1.94017 factor:1 | 1 (-1.47937) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.62160 HOMO: -6.80829 LUMO: 1.78507 factor:1 | 1 (-1.16487) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04512 HOMO: -6.58243 LUMO: 1.78235 factor:1 | 1 (-1.58838) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91153 HOMO: -5.85045 LUMO: 1.82316 factor:1 | 1 (-1.45480) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96087 HOMO: -5.93752 LUMO: 1.56465 factor:1 | 1 (-1.50414) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87172 HOMO: -6.59604 LUMO: -0.53334 factor:1 | 1 (-1.41499) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92000 HOMO: -7.06135 LUMO: 0.29660 factor:1 | 1 (-1.46327) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84560 HOMO: -6.50352 LUMO: 1.61908 factor:1 | 1 (-1.38887) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.60364 HOMO: -6.68040 LUMO: -0.60681 factor:1 | 1 (-1.14691) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.73325 HOMO: -6.93618 LUMO: -1.09662 factor:1 | 1 (-1.27651) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52173 HOMO: -6.72121 LUMO: -1.14016 factor:1 | 1 (-1.06500) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89953 HOMO: -7.12394 LUMO: -1.24900 factor:1 | 1 (-2.44279) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.63043 HOMO: -6.71305 LUMO: -0.71566 factor:1 | 1 (-2.17370) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56167 HOMO: -7.09401 LUMO: -0.86532 factor:1 | 1 (-2.10494) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48286 HOMO: -7.08584 LUMO: -0.92519 factor:1 | 1 (-3.02612) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.17120 HOMO: -7.05591 LUMO: 0.11973 factor:1 | 1 (-3.71446) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.30905 HOMO: -7.14843 LUMO: -1.58370 factor:1 | 1 (-3.85232) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37243 HOMO: -7.36884 LUMO: -1.97010 factor:1 | 1 (-2.91570) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.32321 HOMO: -6.81373 LUMO: -1.72248 factor:1 | 1 (-2.86647) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52593 HOMO: -6.87360 LUMO: -1.03947 factor:1 | 1 (-3.06920) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.09813 HOMO: -7.02870 LUMO: -0.87349 factor:1 | 1 (-3.64140) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.96129 HOMO: -7.16476 LUMO: -1.18097 factor:1 | 1 (-3.50455) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.13846 HOMO: -7.51851 LUMO: 0.07891 factor:1 | 1 (-3.68173) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.45589 HOMO: -7.04231 LUMO: -0.83539 factor:1 | 1 (-2.99916) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.12113 HOMO: -6.83278 LUMO: -0.60137 factor:1 | 1 (-3.66439) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.58731 HOMO: -6.89809 LUMO: -1.19186 factor:1 | 1 (-4.13058) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46388 HOMO: -7.16476 LUMO: -0.79185 factor:1 | 1 (-1.00715) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45544 HOMO: -6.97156 LUMO: -1.25444 factor:1 | 1 (-1.99870) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22528 HOMO: -6.84366 LUMO: -0.88437 factor:1 | 1 (-1.76855) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.17193 HOMO: -6.91986 LUMO: -1.12655 factor:1 | 1 (-3.71520) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.49543 HOMO: -6.49536 LUMO: -0.29660 factor:1 | 1 (-3.03870) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.37136 HOMO: -6.74842 LUMO: 0.42450 factor:1 | 1 (-3.91463) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79645 HOMO: -7.34435 LUMO: 0.32109 factor:1 | 1 (-2.33972) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.40002 HOMO: -7.16476 LUMO: 0.28572 factor:1 | 1 (-0.94328) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.52273 HOMO: -6.74298 LUMO: -0.43538 factor:1 | 1 (-2.06600) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50248 HOMO: -7.19469 LUMO: -1.61091 factor:1 | 1 (-2.04575) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40896 HOMO: -7.35252 LUMO: -1.78235 factor:1 | 1 (-1.95223) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53791 HOMO: -7.25456 LUMO: -1.66806 factor:1 | 1 (-2.08118) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92102 HOMO: -7.54844 LUMO: -1.07213 factor:1 | 1 (-2.46429) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50765 HOMO: -7.21918 LUMO: -1.55377 factor:1 | 1 (-2.05092) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.31839 HOMO: -7.01782 LUMO: -1.60547 factor:1 | 1 (-2.86166) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.31583 HOMO: -7.21646 LUMO: -1.53472 factor:1 | 1 (-2.85910) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52610 HOMO: -6.73754 LUMO: -1.37417 factor:1 | 1 (-3.06936) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.28930 HOMO: -6.78924 LUMO: 0.66396 factor:1 | 1 (-2.83257) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65620 HOMO: -6.82734 LUMO: 0.61226 factor:1 | 1 (-2.19947) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99082 HOMO: -6.74026 LUMO: 0.65579 factor:1 | 1 (-2.53409) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12658 HOMO: -7.10489 LUMO: -1.30887 factor:1 | 1 (-2.66985) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99175 HOMO: -7.05047 LUMO: 0.42722 factor:1 | 1 (-2.53501) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44431 HOMO: -6.61237 LUMO: 1.30887 factor:1 | 1 (-1.98757) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58355 HOMO: -7.05863 LUMO: 0.59049 factor:1 | 1 (-2.12681) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67383 HOMO: -6.26406 LUMO: 0.78641 factor:1 | 1 (-2.21710) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.56475 HOMO: -6.70489 LUMO: 0.67756 factor:1 | 1 (-1.10802) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26932 HOMO: -6.78652 LUMO: -0.94968 factor:1 | 1 (-0.81259) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83972 HOMO: -6.36202 LUMO: -0.94424 factor:1 | 1 (-2.38298) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26192 HOMO: -6.81645 LUMO: -1.09934 factor:1 | 1 (-0.80518) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.95792 HOMO: -7.07224 LUMO: 0.85988 factor:1 | 1 (-2.50119) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96358 HOMO: -7.02326 LUMO: 1.10206 factor:1 | 1 (-2.50685) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.29568 HOMO: -6.71305 LUMO: 0.84627 factor:1 | 1 (-1.83895) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.43312 HOMO: -7.27360 LUMO: 0.88165 factor:1 | 1 (-1.97639) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17391 HOMO: -6.84911 LUMO: 0.59865 factor:1 | 1 (-1.71717) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18406 HOMO: -6.75114 LUMO: -2.49801 factor:1 | 1 (-1.72732) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13758 HOMO: -6.97156 LUMO: 0.53606 factor:1 | 1 (-1.68085) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16479 HOMO: -6.54434 LUMO: 0.73199 factor:1 | 1 (-1.70806) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.13188 HOMO: -6.21236 LUMO: 0.99866 factor:1 | 1 (-3.67514) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.35163 HOMO: -6.34025 LUMO: 0.50341 factor:1 | 1 (-3.89490) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.95448 HOMO: -6.59876 LUMO: -0.69389 factor:1 | 1 (-3.49775) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.40231 HOMO: -6.54978 LUMO: -1.00682 factor:1 | 1 (-2.94558) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90943 HOMO: -6.82462 LUMO: -0.98777 factor:1 | 1 (-2.45270) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65658 HOMO: -6.85455 LUMO: -0.68573 factor:1 | 1 (-2.19985) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46491 HOMO: -7.55388 LUMO: -0.03265 factor:1 | 1 (-1.00818) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48987 HOMO: -6.77019 LUMO: -0.71838 factor:1 | 1 (-1.03313) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50251 HOMO: -6.84911 LUMO: -1.25444 factor:1 | 1 (-2.04578) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45789 HOMO: -6.95251 LUMO: -1.03675 factor:1 | 1 (-2.00115) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37499 HOMO: -6.80829 LUMO: -0.77280 factor:1 | 1 (-2.91826) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93501 HOMO: -6.94162 LUMO: -0.94151 factor:1 | 1 (-2.47828) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.98151 HOMO: -6.89809 LUMO: -0.90886 factor:1 | 1 (-2.52478) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03251 HOMO: -6.85183 LUMO: -0.88981 factor:1 | 1 (-2.57578) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88943 HOMO: -6.51985 LUMO: -0.84627 factor:1 | 1 (-2.43270) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93950 HOMO: -6.83278 LUMO: -1.08029 factor:1 | 1 (-2.48277) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35462 HOMO: -6.91986 LUMO: 0.66396 factor:1 | 1 (-1.89789) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36714 HOMO: -6.94162 LUMO: 0.50885 factor:1 | 1 (-1.91040) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87041 HOMO: -6.94435 LUMO: 0.80546 factor:1 | 1 (-2.41368) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96310 HOMO: -6.74298 LUMO: -0.81634 factor:1 | 1 (-1.50637) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79710 HOMO: -7.04503 LUMO: 1.15921 factor:1 | 1 (-2.34037) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36649 HOMO: -6.76475 LUMO: 0.75920 factor:1 | 1 (-0.90976) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29909 HOMO: -7.05047 LUMO: 0.68845 factor:1 | 1 (-0.84236) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24926 HOMO: -7.12666 LUMO: 0.60681 factor:1 | 1 (-0.79253) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.11386 HOMO: -6.90897 LUMO: -1.22723 factor:1 | 1 (-0.65713) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65636 HOMO: -7.10761 LUMO: 0.58232 factor:1 | 1 (-2.19963) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11158 HOMO: -6.57427 LUMO: 0.71294 factor:1 | 1 (-2.65485) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21375 HOMO: -6.22597 LUMO: 0.99322 factor:1 | 1 (-0.75702) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96359 HOMO: -6.83550 LUMO: -0.77825 factor:1 | 1 (-1.50686) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71280 HOMO: -7.14843 LUMO: 0.44627 factor:1 | 1 (-2.25607) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83849 HOMO: -7.08040 LUMO: 0.78913 factor:1 | 1 (-2.38176) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92521 HOMO: -6.81373 LUMO: -0.93879 factor:1 | 1 (-2.46848) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24126 HOMO: -6.95251 LUMO: 0.22585 factor:1 | 1 (-1.78452) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.60239 HOMO: -7.13483 LUMO: -1.25444 factor:1 | 1 (-1.14565) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29014 HOMO: -6.37835 LUMO: -1.54289 factor:1 | 1 (-0.83340) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.68124 HOMO: -6.53617 LUMO: -1.43948 factor:1 | 1 (-1.22451) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44622 HOMO: -6.38379 LUMO: 0.16055 factor:1 | 1 (-0.98949) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48192 HOMO: -6.53617 LUMO: 0.15783 factor:1 | 1 (-1.02519) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11249 HOMO: -6.79740 LUMO: -0.17960 factor:1 | 1 (-1.65576) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90008 HOMO: -6.26678 LUMO: -0.41361 factor:1 | 1 (-1.44335) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39686 HOMO: -6.35658 LUMO: -0.24218 factor:1 | 1 (-0.94013) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99897 HOMO: -6.48175 LUMO: -0.71566 factor:1 | 1 (-1.54223) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98465 HOMO: -6.21508 LUMO: -0.40001 factor:1 | 1 (-1.52792) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89777 HOMO: -6.51985 LUMO: -0.32654 factor:1 | 1 (-1.44103) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95110 HOMO: -6.45182 LUMO: -0.66396 factor:1 | 1 (-1.49437) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98846 HOMO: -6.51441 LUMO: -0.65307 factor:1 | 1 (-1.53173) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95695 HOMO: -6.57971 LUMO: -0.92519 factor:1 | 1 (-1.50022) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.72609 HOMO: -6.67223 LUMO: -0.58232 factor:1 | 1 (-1.26936) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83183 HOMO: -6.10351 LUMO: -0.45987 factor:1 | 1 (-1.37510) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33337 HOMO: -6.13889 LUMO: -0.50341 factor:1 | 1 (-1.87663) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19328 HOMO: -6.63141 LUMO: -0.28300 factor:1 | 1 (-1.73655) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.40663 HOMO: -6.37563 LUMO: -0.22858 factor:1 | 1 (-0.94990) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15860 HOMO: -6.37019 LUMO: 0.11429 factor:1 | 1 (-0.70186) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21857 HOMO: -6.23957 LUMO: 0.28844 factor:1 | 1 (-0.76184) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20834 HOMO: -6.41372 LUMO: -0.53879 factor:1 | 1 (-0.75161) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.17754 HOMO: -7.06680 LUMO: 0.32654 factor:1 | 1 (-0.72080) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.08834 HOMO: -6.50896 LUMO: -0.73743 factor:1 | 1 (-0.63160) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32369 HOMO: -6.42189 LUMO: -0.28572 factor:1 | 1 (-0.86695) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16401 HOMO: -6.79740 LUMO: -0.25851 factor:1 | 1 (-0.70728) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89379 HOMO: -6.32393 LUMO: 0.17960 factor:1 | 1 (-1.43706) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99709 HOMO: -6.65046 LUMO: 0.03537 factor:1 | 1 (-1.54035) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85186 HOMO: -6.60148 LUMO: 0.07619 factor:1 | 1 (-1.39513) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95094 HOMO: -6.57971 LUMO: 0.11429 factor:1 | 1 (-1.49420) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.83870 HOMO: -6.88448 LUMO: -1.21907 factor:1 | 1 (-0.38197) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.83818 HOMO: -6.97700 LUMO: 0.36463 factor:1 | 1 (-0.38145) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22006 HOMO: -6.73210 LUMO: -0.84083 factor:1 | 1 (-1.76333) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10108 HOMO: -6.21236 LUMO: -0.68845 factor:1 | 1 (-2.64435) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.21779 HOMO: -6.35658 LUMO: -0.82995 factor:1 | 1 (-2.76106) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.84180 HOMO: -6.75114 LUMO: -0.94424 factor:1 | 1 (-0.38507) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.77397 HOMO: -6.74026 LUMO: -1.46125 factor:1 | 1 (-2.31724) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91170 HOMO: -7.06952 LUMO: 0.91974 factor:1 | 1 (-1.45497) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62646 HOMO: -7.08857 LUMO: 0.74559 factor:1 | 1 (-2.16973) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83118 HOMO: -6.74298 LUMO: 1.03131 factor:1 | 1 (-1.37445) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87894 HOMO: -6.74842 LUMO: -1.77962 factor:1 | 1 (-1.42220) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.64260 HOMO: -6.82462 LUMO: -1.61908 factor:1 | 1 (-1.18587) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53651 HOMO: -7.17020 LUMO: -1.02043 factor:1 | 1 (-1.07978) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48418 HOMO: -6.26406 LUMO: -0.96328 factor:1 | 1 (-1.02745) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57117 HOMO: -6.50896 LUMO: -0.38640 factor:1 | 1 (-1.11444) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17500 HOMO: -7.27632 LUMO: -1.17553 factor:1 | 1 (-1.71826) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24885 HOMO: -6.54162 LUMO: -1.36873 factor:1 | 1 (-1.79211) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57353 HOMO: -6.42733 LUMO: -1.15648 factor:1 | 1 (-2.11680) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25187 HOMO: -6.73754 LUMO: -2.58780 factor:1 | 1 (-1.79514) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74263 HOMO: -7.20285 LUMO: 0.75103 factor:1 | 1 (-1.28590) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.59893 HOMO: -6.98788 LUMO: 0.34831 factor:1 | 1 (-1.14220) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.59275 HOMO: -6.80013 LUMO: -1.11567 factor:1 | 1 (-1.13602) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90056 HOMO: -6.67767 LUMO: -0.82450 factor:1 | 1 (-2.44383) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.85259 HOMO: -6.84911 LUMO: -0.21497 factor:1 | 1 (-2.39585) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50121 HOMO: -6.23141 LUMO: 0.21769 factor:1 | 1 (-2.04447) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.20487 HOMO: -6.68312 LUMO: 0.16327 factor:1 | 1 (-1.74814) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09989 HOMO: -7.04503 LUMO: -1.04220 factor:1 | 1 (-1.64316) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18321 HOMO: -6.67495 LUMO: -0.71294 factor:1 | 1 (-1.72648) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12264 HOMO: -6.70216 LUMO: -0.55239 factor:1 | 1 (-1.66591) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46306 HOMO: -6.60420 LUMO: -0.71294 factor:1 | 1 (-1.00633) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.21772 HOMO: -7.40694 LUMO: 0.11973 factor:1 | 1 (-1.76098) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44508 HOMO: -6.58788 LUMO: -0.29116 factor:1 | 1 (-0.98834) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.66658 HOMO: -6.63686 LUMO: -0.32654 factor:1 | 1 (-1.20985) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34899 HOMO: -6.85183 LUMO: -0.95512 factor:1 | 1 (-0.89226) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.51131 HOMO: -6.82189 LUMO: -0.88165 factor:1 | 1 (-1.05458) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.50960 HOMO: -6.97428 LUMO: -1.03947 factor:1 | 1 (-1.05286) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29759 HOMO: -6.51441 LUMO: -0.05714 factor:1 | 1 (-0.84086) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.31865 HOMO: -6.61509 LUMO: -0.77008 factor:1 | 1 (-0.86192) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58481 HOMO: -7.36340 LUMO: 0.29116 factor:1 | 1 (-1.12808) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00476 HOMO: -6.64230 LUMO: -0.79185 factor:1 | 1 (-1.54803) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14425 HOMO: -6.56883 LUMO: -1.03403 factor:1 | 1 (-1.68751) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04049 HOMO: -6.69400 LUMO: -0.77825 factor:1 | 1 (-1.58376) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48168 HOMO: -6.37019 LUMO: -0.79185 factor:1 | 1 (-1.02494) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.60941 HOMO: -6.49808 LUMO: -0.94424 factor:1 | 1 (-1.15267) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.64856 HOMO: -6.91713 LUMO: -0.75376 factor:1 | 1 (-2.19182) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65577 HOMO: -7.13755 LUMO: 0.41361 factor:1 | 1 (-2.19903) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41448 HOMO: -7.12122 LUMO: 0.39457 factor:1 | 1 (-1.95775) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97910 HOMO: -6.59332 LUMO: -0.57144 factor:1 | 1 (-1.52237) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.59928 HOMO: -6.62325 LUMO: -0.66940 factor:1 | 1 (-1.14255) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75019 HOMO: -6.90897 LUMO: -0.08708 factor:1 | 1 (-2.29346) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72516 HOMO: -6.65591 LUMO: -0.81090 factor:1 | 1 (-2.26842) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69296 HOMO: -6.65318 LUMO: -0.94696 factor:1 | 1 (-2.23623) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53726 HOMO: -6.96067 LUMO: -1.03675 factor:1 | 1 (-2.08053) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84064 HOMO: -6.23141 LUMO: -0.66396 factor:1 | 1 (-2.38391) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65900 HOMO: -6.52529 LUMO: -0.78369 factor:1 | 1 (-2.20227) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80399 HOMO: -6.39468 LUMO: -0.40817 factor:1 | 1 (-2.34725) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59370 HOMO: -6.76203 LUMO: -0.20409 factor:1 | 1 (-2.13696) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96656 HOMO: -6.96611 LUMO: -0.90342 factor:1 | 1 (-1.50982) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13181 HOMO: -6.54706 LUMO: -0.87893 factor:1 | 1 (-1.67508) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28335 HOMO: -7.24367 LUMO: -0.97689 factor:1 | 1 (-1.82662) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14686 HOMO: -6.61781 LUMO: 1.43404 factor:1 | 1 (-1.69013) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45818 HOMO: -6.17971 LUMO: 1.79867 factor:1 | 1 (-2.00145) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12920 HOMO: -5.73344 LUMO: 2.13609 factor:1 | 1 (-1.67247) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93759 HOMO: -6.72121 LUMO: 2.06807 factor:1 | 1 (-2.48086) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84323 HOMO: -6.91169 LUMO: 2.02997 factor:1 | 1 (-2.38649) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84344 HOMO: -7.06408 LUMO: 1.41499 factor:1 | 1 (-2.38671) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72733 HOMO: -6.94162 LUMO: -0.90070 factor:1 | 1 (-2.27060) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71226 HOMO: -7.09401 LUMO: 0.35103 factor:1 | 1 (-2.25552) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48923 HOMO: -6.78652 LUMO: 0.91974 factor:1 | 1 (-2.03250) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.66213 HOMO: -6.32937 LUMO: -1.89119 factor:1 | 1 (-2.20540) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39693 HOMO: -7.12666 LUMO: -1.06397 factor:1 | 1 (-1.94020) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48186 HOMO: -6.38107 LUMO: -1.43132 factor:1 | 1 (-2.02513) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65272 HOMO: -7.09129 LUMO: 0.08980 factor:1 | 1 (-2.19599) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65824 HOMO: -6.31304 LUMO: -0.57960 factor:1 | 1 (-2.20151) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58798 HOMO: -6.94435 LUMO: -0.74287 factor:1 | 1 (-2.13125) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.77601 HOMO: -6.35658 LUMO: -1.53472 factor:1 | 1 (-2.31928) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73014 HOMO: -6.39740 LUMO: -1.48846 factor:1 | 1 (-2.27340) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33897 HOMO: -7.05319 LUMO: -0.33198 factor:1 | 1 (-1.88224) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08716 HOMO: -6.68040 LUMO: -0.09252 factor:1 | 1 (-1.63042) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28224 HOMO: -6.35930 LUMO: -0.43266 factor:1 | 1 (-1.82550) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30694 HOMO: -6.59604 LUMO: -1.45853 factor:1 | 1 (-1.85021) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.21391 HOMO: -6.46270 LUMO: -1.49391 factor:1 | 1 (-1.75718) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16177 HOMO: -7.05863 LUMO: -1.04764 factor:1 | 1 (-1.70504) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17600 HOMO: -7.14027 LUMO: -0.81634 factor:1 | 1 (-1.71927) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18885 HOMO: -6.80285 LUMO: -0.74287 factor:1 | 1 (-1.73211) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89114 HOMO: -6.53890 LUMO: -1.13471 factor:1 | 1 (-2.43441) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.86004 HOMO: -6.49808 LUMO: -1.35513 factor:1 | 1 (-2.40331) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07295 HOMO: -6.75931 LUMO: -1.49663 factor:1 | 1 (-1.61622) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15358 HOMO: -6.84638 LUMO: -0.77552 factor:1 | 1 (-1.69685) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.65412 HOMO: -6.65863 LUMO: -1.34696 factor:1 | 1 (-1.19738) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10887 HOMO: -6.25590 LUMO: -2.36467 factor:1 | 1 (-1.65214) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75476 HOMO: -7.24911 LUMO: 0.33470 factor:1 | 1 (-2.29803) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.28955 HOMO: -6.65863 LUMO: -0.75648 factor:1 | 1 (-2.83281) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.77078 HOMO: -6.31576 LUMO: -0.83267 factor:1 | 1 (-3.31405) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.77043 HOMO: -6.64774 LUMO: -0.66124 factor:1 | 1 (-3.31369) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.87111 HOMO: -6.75387 LUMO: -1.00138 factor:1 | 1 (-3.41438) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29801 HOMO: -6.52529 LUMO: -0.68301 factor:1 | 1 (-2.84128) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.50041 HOMO: -6.59332 LUMO: -0.68028 factor:1 | 1 (-3.04368) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.91244 HOMO: -5.98650 LUMO: 0.31565 factor:1 | 1 (-3.45571) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.50199 HOMO: -6.59876 LUMO: 0.22585 factor:1 | 1 (-3.04525) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.04134 HOMO: -6.72121 LUMO: 0.10340 factor:1 | 1 (-3.58461) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30005 HOMO: -6.09807 LUMO: 0.20136 factor:1 | 1 (-2.84332) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.79747 HOMO: -6.31576 LUMO: 0.06259 factor:1 | 1 (-3.34074) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.84050 HOMO: -6.35658 LUMO: -0.58232 factor:1 | 1 (-3.38376) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.12725 HOMO: -6.34842 LUMO: -0.55783 factor:1 | 1 (-3.67052) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.90270 HOMO: -6.47359 LUMO: -0.57144 factor:1 | 1 (-3.44597) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23512 HOMO: -6.42189 LUMO: -0.09796 factor:1 | 1 (-2.77839) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.72558 HOMO: -6.35658 LUMO: -0.31293 factor:1 | 1 (-3.26885) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48778 HOMO: -7.35524 LUMO: 0.10340 factor:1 | 1 (-3.03105) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29659 HOMO: -7.10217 LUMO: 0.36463 factor:1 | 1 (-2.83986) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.42117 HOMO: -6.43549 LUMO: -0.56872 factor:1 | 1 (-2.96444) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30571 HOMO: -6.50080 LUMO: -0.71294 factor:1 | 1 (-2.84898) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96056 HOMO: -6.59060 LUMO: -0.57960 factor:1 | 1 (-2.50383) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10065 HOMO: -6.78924 LUMO: -0.31565 factor:1 | 1 (-2.64391) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11431 HOMO: -6.35658 LUMO: 0.07891 factor:1 | 1 (-2.65757) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15066 HOMO: -6.74026 LUMO: -0.87621 factor:1 | 1 (-2.69393) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20723 HOMO: -6.54434 LUMO: 0.81906 factor:1 | 1 (-2.75050) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23654 HOMO: -6.66135 LUMO: 1.40955 factor:1 | 1 (-2.77981) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.00091 HOMO: -6.73754 LUMO: -2.54971 factor:1 | 1 (-3.54417) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.73165 HOMO: -6.65318 LUMO: 0.69389 factor:1 | 1 (-3.27492) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.96580 HOMO: -6.73482 LUMO: 0.62858 factor:1 | 1 (-3.50907) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25042 HOMO: -6.83550 LUMO: 0.68573 factor:1 | 1 (-2.79368) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.34876 HOMO: -6.83278 LUMO: 0.45987 factor:1 | 1 (-2.89203) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92528 HOMO: -6.78380 LUMO: 0.68301 factor:1 | 1 (-1.46854) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04046 HOMO: -6.90625 LUMO: 1.36601 factor:1 | 1 (-1.58373) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79136 HOMO: -6.82734 LUMO: 1.48302 factor:1 | 1 (-2.33463) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87267 HOMO: -6.44094 LUMO: -0.94424 factor:1 | 1 (-2.41594) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15334 HOMO: -6.91441 LUMO: 0.28844 factor:1 | 1 (-1.69660) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30003 HOMO: -6.49808 LUMO: -0.51157 factor:1 | 1 (-1.84330) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25678 HOMO: -7.09673 LUMO: -0.06259 factor:1 | 1 (-2.80005) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.21970 HOMO: -6.77019 LUMO: 0.92247 factor:1 | 1 (-2.76296) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29034 HOMO: -6.75931 LUMO: 1.13744 factor:1 | 1 (-2.83360) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92988 HOMO: -6.15794 LUMO: 1.12383 factor:1 | 1 (-1.47314) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06490 HOMO: -6.59604 LUMO: 1.19458 factor:1 | 1 (-1.60817) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86846 HOMO: -7.09401 LUMO: 0.60137 factor:1 | 1 (-1.41173) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83781 HOMO: -6.34025 LUMO: 0.48164 factor:1 | 1 (-2.38108) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76807 HOMO: -6.72665 LUMO: -2.47624 factor:1 | 1 (-2.31134) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90227 HOMO: -6.48175 LUMO: 0.58232 factor:1 | 1 (-2.44554) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02304 HOMO: -6.94162 LUMO: 0.28300 factor:1 | 1 (-2.56631) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79120 HOMO: -6.65591 LUMO: 0.57144 factor:1 | 1 (-2.33446) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83381 HOMO: -6.58788 LUMO: -1.03947 factor:1 | 1 (-2.37708) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99351 HOMO: -7.18108 LUMO: 0.37824 factor:1 | 1 (-2.53678) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92878 HOMO: -6.63958 LUMO: -1.52112 factor:1 | 1 (-2.47205) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.53137 HOMO: -6.12528 LUMO: -0.53606 factor:1 | 1 (-3.07464) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.86368 HOMO: -6.22324 LUMO: -0.87893 factor:1 | 1 (-3.40695) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.73358 HOMO: -6.62053 LUMO: -0.91974 factor:1 | 1 (-3.27685) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06429 HOMO: -6.84366 LUMO: -0.83811 factor:1 | 1 (-2.60756) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.08701 HOMO: -7.26000 LUMO: 0.25851 factor:1 | 1 (-2.63028) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58389 HOMO: -6.49536 LUMO: -0.63403 factor:1 | 1 (-3.12716) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88110 HOMO: -6.45726 LUMO: -0.77825 factor:1 | 1 (-2.42437) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73476 HOMO: -6.74570 LUMO: -0.75103 factor:1 | 1 (-2.27803) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80453 HOMO: -7.20285 LUMO: 0.10612 factor:1 | 1 (-2.34780) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60711 HOMO: -6.45182 LUMO: -0.56600 factor:1 | 1 (-2.15038) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.35204 HOMO: -6.83278 LUMO: -0.71838 factor:1 | 1 (-0.89531) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.27784 HOMO: -7.01510 LUMO: -1.09662 factor:1 | 1 (-0.82110) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.56007 HOMO: -6.48719 LUMO: 0.16871 factor:1 | 1 (-1.10334) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30390 HOMO: -7.30898 LUMO: 0.26667 factor:1 | 1 (-1.84716) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99030 HOMO: -6.68856 LUMO: -0.78641 factor:1 | 1 (-2.53357) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81920 HOMO: -6.56883 LUMO: -1.00682 factor:1 | 1 (-2.36247) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45037 HOMO: -6.41100 LUMO: -0.48980 factor:1 | 1 (-1.99364) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48303 HOMO: -6.52257 LUMO: -0.59865 factor:1 | 1 (-2.02630) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45427 HOMO: -6.63686 LUMO: -0.56055 factor:1 | 1 (-0.99754) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45193 HOMO: -6.79740 LUMO: -0.75376 factor:1 | 1 (-0.99520) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58043 HOMO: -5.89127 LUMO: 0.22313 factor:1 | 1 (-1.12369) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03197 HOMO: -6.34842 LUMO: 0.11429 factor:1 | 1 (-1.57524) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14082 HOMO: -6.13617 LUMO: 1.94834 factor:1 | 1 (-1.68409) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98449 HOMO: -6.50080 LUMO: 1.74153 factor:1 | 1 (-1.52776) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.47262 HOMO: -6.33481 LUMO: 1.68438 factor:1 | 1 (-1.01588) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.50034 HOMO: -6.53073 LUMO: 1.95106 factor:1 | 1 (-1.04361) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.41215 HOMO: -6.46270 LUMO: 1.89935 factor:1 | 1 (-0.95542) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10246 HOMO: -5.87222 LUMO: 1.91568 factor:1 | 1 (-0.64573) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.52395 HOMO: -6.07630 LUMO: 1.81500 factor:1 | 1 (-2.06722) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33709 HOMO: -6.20964 LUMO: 1.81500 factor:1 | 1 (-2.88035) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.26326 HOMO: -6.15522 LUMO: 1.90752 factor:1 | 1 (-2.80653) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.17261 HOMO: -6.11984 LUMO: 1.95378 factor:1 | 1 (-0.71588) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65367 HOMO: -6.58516 LUMO: 2.04358 factor:1 | 1 (-2.19694) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65830 HOMO: -7.37156 LUMO: 0.24490 factor:1 | 1 (-2.20156) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97205 HOMO: -6.36474 LUMO: -0.90070 factor:1 | 1 (-1.51532) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75718 HOMO: -6.43549 LUMO: -0.40817 factor:1 | 1 (-2.30045) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07176 HOMO: -7.32258 LUMO: 0.29388 factor:1 | 1 (-1.61502) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18104 HOMO: -6.41372 LUMO: -0.20409 factor:1 | 1 (-1.72430) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16109 HOMO: -7.18381 LUMO: 0.42722 factor:1 | 1 (-1.70436) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16476 HOMO: -6.53890 LUMO: -0.54151 factor:1 | 1 (-1.70803) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26278 HOMO: -6.61509 LUMO: 0.08708 factor:1 | 1 (-1.80605) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13875 HOMO: -6.78108 LUMO: 2.03541 factor:1 | 1 (-1.68202) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04691 HOMO: -6.50896 LUMO: 1.53472 factor:1 | 1 (-1.59018) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14016 HOMO: -6.65591 LUMO: 1.80411 factor:1 | 1 (-1.68343) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12095 HOMO: -6.64502 LUMO: 1.52112 factor:1 | 1 (-1.66422) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05502 HOMO: -6.72938 LUMO: 1.48030 factor:1 | 1 (-1.59829) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26006 HOMO: -6.16882 LUMO: 1.96466 factor:1 | 1 (-1.80333) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05350 HOMO: -6.22597 LUMO: 1.43132 factor:1 | 1 (-1.59676) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08523 HOMO: -6.57699 LUMO: 2.05718 factor:1 | 1 (-1.62849) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09777 HOMO: -6.52529 LUMO: 1.89663 factor:1 | 1 (-1.64104) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94922 HOMO: -6.30760 LUMO: 1.88031 factor:1 | 1 (-1.49249) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82302 HOMO: -6.14977 LUMO: 1.92657 factor:1 | 1 (-1.36628) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04746 HOMO: -6.20964 LUMO: 1.83949 factor:1 | 1 (-1.59072) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82310 HOMO: -6.31848 LUMO: 1.91296 factor:1 | 1 (-1.36637) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14226 HOMO: -5.80691 LUMO: 2.19868 factor:1 | 1 (-1.68553) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42232 HOMO: -6.00827 LUMO: 2.15514 factor:1 | 1 (-1.96559) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99584 HOMO: -6.51713 LUMO: 2.08711 factor:1 | 1 (-1.53910) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99858 HOMO: -6.32937 LUMO: 2.11705 factor:1 | 1 (-1.54185) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.69120 HOMO: -6.26678 LUMO: 1.95922 factor:1 | 1 (-1.23447) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04898 HOMO: -6.43005 LUMO: 2.56603 factor:1 | 1 (-1.59225) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10950 HOMO: -6.41644 LUMO: 2.68304 factor:1 | 1 (-1.65277) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25317 HOMO: -5.97834 LUMO: 2.02997 factor:1 | 1 (-1.79644) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12248 HOMO: -6.14161 LUMO: 1.77690 factor:1 | 1 (-1.66574) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68709 HOMO: -6.21508 LUMO: 1.80411 factor:1 | 1 (-2.23035) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67615 HOMO: -6.46270 LUMO: 2.34562 factor:1 | 1 (-2.21942) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.95093 HOMO: -6.39195 LUMO: -0.75920 factor:1 | 1 (-2.49420) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.95422 HOMO: -7.08584 LUMO: -1.14016 factor:1 | 1 (-2.49749) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80363 HOMO: -6.70216 LUMO: -0.65035 factor:1 | 1 (-2.34690) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94010 HOMO: -6.79468 LUMO: -0.83811 factor:1 | 1 (-2.48337) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53753 HOMO: -6.99877 LUMO: -0.79729 factor:1 | 1 (-2.08080) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10596 HOMO: -7.08040 LUMO: -0.85444 factor:1 | 1 (-1.64923) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01905 HOMO: -7.39333 LUMO: 0.12789 factor:1 | 1 (-1.56231) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.64907 HOMO: -7.05047 LUMO: 0.13878 factor:1 | 1 (-2.19234) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71925 HOMO: -6.90897 LUMO: -0.77552 factor:1 | 1 (-2.26252) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78200 HOMO: -7.25456 LUMO: 0.05170 factor:1 | 1 (-2.32527) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50937 HOMO: -6.84638 LUMO: -0.84355 factor:1 | 1 (-2.05264) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87297 HOMO: -6.78108 LUMO: -0.81634 factor:1 | 1 (-2.41624) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.72702 HOMO: -6.74570 LUMO: -0.77280 factor:1 | 1 (-3.27029) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13624 HOMO: -7.28177 LUMO: -1.68438 factor:1 | 1 (-2.67951) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.75655 HOMO: -7.22190 LUMO: -1.63540 factor:1 | 1 (-3.29982) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.00075 HOMO: -7.15932 LUMO: -1.57554 factor:1 | 1 (-2.54402) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.17031 HOMO: -6.57971 LUMO: -0.93063 factor:1 | 1 (-2.71357) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.79415 HOMO: -6.88176 LUMO: 0.58232 factor:1 | 1 (-3.33742) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39894 HOMO: -6.85727 LUMO: 0.51430 factor:1 | 1 (-2.94220) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.78569 HOMO: -6.83550 LUMO: 0.87893 factor:1 | 1 (-3.32896) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48101 HOMO: -7.06680 LUMO: 0.87621 factor:1 | 1 (-3.02427) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.75611 HOMO: -6.52257 LUMO: 0.81362 factor:1 | 1 (-3.29938) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58561 HOMO: -6.95523 LUMO: 1.17009 factor:1 | 1 (-3.12887) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84445 HOMO: -7.21374 LUMO: 0.97145 factor:1 | 1 (-2.38772) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.35355 HOMO: -6.81373 LUMO: -1.54561 factor:1 | 1 (-2.89682) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.95860 HOMO: -6.86543 LUMO: -1.52656 factor:1 | 1 (-2.50187) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99852 HOMO: -6.90081 LUMO: -0.78097 factor:1 | 1 (-2.54179) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.40917 HOMO: -6.64502 LUMO: -0.82723 factor:1 | 1 (-2.95244) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.53524 HOMO: -6.65591 LUMO: -0.82178 factor:1 | 1 (-3.07851) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.31306 HOMO: -6.79468 LUMO: -1.46397 factor:1 | 1 (-2.85632) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30677 HOMO: -7.25728 LUMO: 0.73743 factor:1 | 1 (-2.85004) | 1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20693 HOMO: -7.00149 LUMO: 1.30070 factor:1 | 1 (-2.75020) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.60982 HOMO: -7.07768 LUMO: 0.78097 factor:1 | 1 (-3.15309) | 1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13178 HOMO: -6.86271 LUMO: 0.86260 factor:1 | 1 (-1.67505) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89694 HOMO: -6.94707 LUMO: 0.39729 factor:1 | 1 (-2.44021) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87207 HOMO: -6.79740 LUMO: 0.67484 factor:1 | 1 (-2.41534) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70935 HOMO: -6.91986 LUMO: -1.14288 factor:1 | 1 (-2.25261) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99006 HOMO: -6.31576 LUMO: 1.01771 factor:1 | 1 (-2.53333) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94832 HOMO: -6.81645 LUMO: 0.81362 factor:1 | 1 (-2.49158) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87928 HOMO: -6.92258 LUMO: -0.99594 factor:1 | 1 (-2.42255) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75590 HOMO: -6.81373 LUMO: 0.61770 factor:1 | 1 (-2.29917) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.98467 HOMO: -7.18653 LUMO: 1.19186 factor:1 | 1 (-2.52794) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88630 HOMO: -7.00693 LUMO: 0.45715 factor:1 | 1 (-2.42957) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97060 HOMO: -7.11306 LUMO: 0.53334 factor:1 | 1 (-2.51387) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97213 HOMO: -6.63414 LUMO: -1.64357 factor:1 | 1 (-2.51539) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13069 HOMO: -6.22052 LUMO: -0.74015 factor:1 | 1 (-2.67395) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94949 HOMO: -6.81101 LUMO: -0.50069 factor:1 | 1 (-1.49276) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88732 HOMO: -6.71849 LUMO: -0.51974 factor:1 | 1 (-1.43058) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90658 HOMO: -6.72121 LUMO: -1.77690 factor:1 | 1 (-1.44985) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74620 HOMO: -6.94162 LUMO: -1.78779 factor:1 | 1 (-1.28947) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11738 HOMO: -6.91169 LUMO: 0.88981 factor:1 | 1 (-2.66065) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.19409 HOMO: -6.97428 LUMO: 0.70750 factor:1 | 1 (-2.73736) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10486 HOMO: -6.74842 LUMO: 1.15921 factor:1 | 1 (-2.64813) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85483 HOMO: -7.25183 LUMO: -0.99594 factor:1 | 1 (-1.39809) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91815 HOMO: -6.43821 LUMO: -1.00410 factor:1 | 1 (-1.46141) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.72906 HOMO: -6.52257 LUMO: -0.68573 factor:1 | 1 (-1.27232) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.72800 HOMO: -6.60148 LUMO: -0.52518 factor:1 | 1 (-3.27127) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.38343 HOMO: -6.07086 LUMO: -1.39594 factor:1 | 1 (-2.92669) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48264 HOMO: -6.78108 LUMO: -1.54833 factor:1 | 1 (-3.02591) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89912 HOMO: -6.73482 LUMO: -1.01498 factor:1 | 1 (-2.44239) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.61325 HOMO: -6.85183 LUMO: 1.06669 factor:1 | 1 (-3.15652) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87384 HOMO: -6.98516 LUMO: 1.43948 factor:1 | 1 (-2.41711) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74733 HOMO: -6.94162 LUMO: 0.79185 factor:1 | 1 (-2.29060) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09597 HOMO: -6.67495 LUMO: -1.06669 factor:1 | 1 (-1.63924) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98612 HOMO: -6.88720 LUMO: -1.00682 factor:1 | 1 (-1.52939) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95616 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-1.49943) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11720 HOMO: -6.51713 LUMO: -0.89798 factor:1 | 1 (-1.66047) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04441 HOMO: -6.63141 LUMO: -0.91430 factor:1 | 1 (-1.58768) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98501 HOMO: -6.63414 LUMO: 0.04354 factor:1 | 1 (-1.52827) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96228 HOMO: -6.65046 LUMO: -0.73743 factor:1 | 1 (-1.50555) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95798 HOMO: -6.73754 LUMO: -0.71838 factor:1 | 1 (-1.50125) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77390 HOMO: -6.65863 LUMO: -0.60137 factor:1 | 1 (-1.31717) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01303 HOMO: -6.61509 LUMO: -0.47892 factor:1 | 1 (-1.55630) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99118 HOMO: -6.82189 LUMO: -0.64763 factor:1 | 1 (-1.53445) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.72486 HOMO: -6.56883 LUMO: -0.51974 factor:1 | 1 (-1.26813) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79600 HOMO: -6.97428 LUMO: -0.95512 factor:1 | 1 (-1.33926) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16248 HOMO: -6.70489 LUMO: -0.04082 factor:1 | 1 (-1.70575) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05085 HOMO: -6.74026 LUMO: 0.02177 factor:1 | 1 (-2.59412) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58670 HOMO: -6.50080 LUMO: -0.89525 factor:1 | 1 (-3.12996) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.88254 HOMO: -6.46815 LUMO: -0.61226 factor:1 | 1 (-3.42580) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.42392 HOMO: -6.57971 LUMO: -0.64219 factor:1 | 1 (-2.96718) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.31314 HOMO: -7.17836 LUMO: 0.37280 factor:1 | 1 (-2.85641) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65973 HOMO: -6.67223 LUMO: 0.12245 factor:1 | 1 (-3.20300) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68512 HOMO: -6.55250 LUMO: 0.22858 factor:1 | 1 (-3.22839) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68901 HOMO: -6.97156 LUMO: -1.12927 factor:1 | 1 (-3.23228) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.00448 HOMO: -6.78924 LUMO: -0.84900 factor:1 | 1 (-2.54775) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97814 HOMO: -6.65046 LUMO: -0.65307 factor:1 | 1 (-2.52141) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96403 HOMO: -7.41782 LUMO: 0.08980 factor:1 | 1 (-1.50729) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91355 HOMO: -6.56339 LUMO: -0.68573 factor:1 | 1 (-1.45682) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04811 HOMO: -6.31032 LUMO: -0.31837 factor:1 | 1 (-1.59138) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06512 HOMO: -6.72938 LUMO: -0.45987 factor:1 | 1 (-1.60838) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83678 HOMO: -6.59876 LUMO: -1.03131 factor:1 | 1 (-2.38004) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62485 HOMO: -7.29265 LUMO: 0.29660 factor:1 | 1 (-2.16812) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91931 HOMO: -6.42189 LUMO: -0.51157 factor:1 | 1 (-2.46258) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87104 HOMO: -6.27767 LUMO: -0.52790 factor:1 | 1 (-2.41430) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83743 HOMO: -6.41644 LUMO: -0.44627 factor:1 | 1 (-2.38070) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89446 HOMO: -6.23413 LUMO: -0.52790 factor:1 | 1 (-2.43773) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90381 HOMO: -6.63414 LUMO: -0.44082 factor:1 | 1 (-1.44707) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.64742 HOMO: -7.03142 LUMO: 0.47076 factor:1 | 1 (-1.19069) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.75458 HOMO: -6.62053 LUMO: -0.14422 factor:1 | 1 (-1.29785) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92993 HOMO: -6.22324 LUMO: 1.96194 factor:1 | 1 (-1.47320) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65448 HOMO: -6.17971 LUMO: 1.71704 factor:1 | 1 (-3.19775) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20467 HOMO: -6.70761 LUMO: 1.68711 factor:1 | 1 (-2.74794) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76409 HOMO: -6.52801 LUMO: 1.56193 factor:1 | 1 (-2.30736) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.47325 HOMO: -6.55794 LUMO: 1.52384 factor:1 | 1 (-3.01652) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72151 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-2.26478) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05779 HOMO: -6.65863 LUMO: 1.83133 factor:1 | 1 (-2.60105) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.51562 HOMO: -6.46270 LUMO: 1.90208 factor:1 | 1 (-3.05889) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14318 HOMO: -6.41917 LUMO: 2.03269 factor:1 | 1 (-2.68644) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15948 HOMO: -6.48992 LUMO: 1.87486 factor:1 | 1 (-2.70274) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88807 HOMO: -6.51985 LUMO: 1.69527 factor:1 | 1 (-2.43134) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89075 HOMO: -6.36202 LUMO: 2.05718 factor:1 | 1 (-1.43401) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53028 HOMO: -5.96474 LUMO: 1.88575 factor:1 | 1 (-1.07354) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44627 HOMO: -6.56339 LUMO: 2.04630 factor:1 | 1 (-0.98954) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15560 HOMO: -6.43277 LUMO: 1.98371 factor:1 | 1 (-0.69887) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33542 HOMO: -6.53345 LUMO: 2.06262 factor:1 | 1 (-0.87868) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44355 HOMO: -5.81779 LUMO: 2.11432 factor:1 | 1 (-0.98682) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52435 HOMO: -5.91848 LUMO: 1.86942 factor:1 | 1 (-3.06762) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.66604 HOMO: -6.48447 LUMO: 1.70343 factor:1 | 1 (-3.20931) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.00349 HOMO: -6.29671 LUMO: -0.89525 factor:1 | 1 (-3.54676) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37047 HOMO: -6.63414 LUMO: -0.76192 factor:1 | 1 (-2.91374) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.63285 HOMO: -6.56883 LUMO: -0.86260 factor:1 | 1 (-3.17611) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.95051 HOMO: -6.93074 LUMO: -0.27483 factor:1 | 1 (-3.49378) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65374 HOMO: -6.85999 LUMO: -0.01905 factor:1 | 1 (-3.19701) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.90352 HOMO: -6.26406 LUMO: 0.21769 factor:1 | 1 (-3.44678) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.26777 HOMO: -6.62325 LUMO: 0.31293 factor:1 | 1 (-3.81104) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39320 HOMO: -6.59604 LUMO: 0.19592 factor:1 | 1 (-1.93647) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47008 HOMO: -6.43277 LUMO: -0.27756 factor:1 | 1 (-2.01334) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97289 HOMO: -6.54978 LUMO: -0.46531 factor:1 | 1 (-2.51616) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05621 HOMO: -6.65046 LUMO: -0.15783 factor:1 | 1 (-2.59948) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.49350 HOMO: -7.28721 LUMO: 0.23946 factor:1 | 1 (-2.03677) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.36498 HOMO: -6.71849 LUMO: -0.56600 factor:1 | 1 (-2.90824) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.99974 HOMO: -6.85183 LUMO: -0.84355 factor:1 | 1 (-3.54300) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.51437 HOMO: -6.53345 LUMO: -0.84627 factor:1 | 1 (-3.05763) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.95623 HOMO: -6.60148 LUMO: -0.63130 factor:1 | 1 (-3.49949) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62224 HOMO: -6.36202 LUMO: -0.60137 factor:1 | 1 (-2.16551) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45437 HOMO: -6.28855 LUMO: -0.52790 factor:1 | 1 (-1.99764) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46627 HOMO: -7.07224 LUMO: 0.41906 factor:1 | 1 (-2.00953) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74042 HOMO: -6.36202 LUMO: -0.24218 factor:1 | 1 (-2.28369) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.26157 HOMO: -6.43549 LUMO: 0.14150 factor:1 | 1 (-2.80484) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18614 HOMO: -6.76747 LUMO: -0.40545 factor:1 | 1 (-2.72941) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.17474 HOMO: -6.15249 LUMO: -0.51157 factor:1 | 1 (-2.71801) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58066 HOMO: -6.33753 LUMO: -0.02993 factor:1 | 1 (-2.12393) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31892 HOMO: -6.49808 LUMO: -0.83811 factor:1 | 1 (-1.86218) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46289 HOMO: -6.64502 LUMO: -0.46259 factor:1 | 1 (-2.00616) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05972 HOMO: -6.34570 LUMO: 0.22041 factor:1 | 1 (-2.60299) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94108 HOMO: -6.63414 LUMO: -0.13606 factor:1 | 1 (-2.48435) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.19684 HOMO: -6.59604 LUMO: -0.79729 factor:1 | 1 (-2.74010) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65122 HOMO: -7.09401 LUMO: 0.31837 factor:1 | 1 (-2.19449) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48335 HOMO: -6.48719 LUMO: -0.31021 factor:1 | 1 (-2.02662) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27826 HOMO: -7.11306 LUMO: 0.39729 factor:1 | 1 (-1.82153) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.01139 HOMO: -6.95251 LUMO: 0.41089 factor:1 | 1 (-2.55466) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79931 HOMO: -6.61509 LUMO: -0.41906 factor:1 | 1 (-2.34257) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12465 HOMO: -6.25318 LUMO: -0.47348 factor:1 | 1 (-2.66791) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.29190 HOMO: -6.77019 LUMO: -0.10340 factor:1 | 1 (-1.83516) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54137 HOMO: -6.54706 LUMO: -0.46259 factor:1 | 1 (-2.08464) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70067 HOMO: -6.34297 LUMO: -0.50341 factor:1 | 1 (-2.24393) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72303 HOMO: -6.20692 LUMO: -0.51974 factor:1 | 1 (-2.26630) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23194 HOMO: -7.03686 LUMO: 0.46804 factor:1 | 1 (-2.77521) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61699 HOMO: -6.47087 LUMO: 0.22585 factor:1 | 1 (-2.16026) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10606 HOMO: -6.41917 LUMO: 0.19320 factor:1 | 1 (-2.64933) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.22174 HOMO: -6.61237 LUMO: -0.04354 factor:1 | 1 (-2.76500) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65519 HOMO: -6.56339 LUMO: 0.36735 factor:1 | 1 (-2.19846) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65386 HOMO: -6.54978 LUMO: 1.12655 factor:1 | 1 (-2.19713) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74317 HOMO: -6.43277 LUMO: 1.17553 factor:1 | 1 (-2.28644) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.26386 HOMO: -6.29944 LUMO: 1.40955 factor:1 | 1 (-2.80713) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.22043 HOMO: -6.74842 LUMO: 0.74015 factor:1 | 1 (-2.76370) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33443 HOMO: -6.15522 LUMO: 1.94289 factor:1 | 1 (-1.87769) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48512 HOMO: -6.20147 LUMO: 1.40139 factor:1 | 1 (-2.02839) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54994 HOMO: -6.41100 LUMO: 1.40139 factor:1 | 1 (-2.09321) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24715 HOMO: -6.74570 LUMO: 1.80956 factor:1 | 1 (-2.79042) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07654 HOMO: -6.60148 LUMO: -1.04764 factor:1 | 1 (-2.61980) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92540 HOMO: -6.82734 LUMO: -0.83267 factor:1 | 1 (-2.46867) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67819 HOMO: -7.01782 LUMO: -0.32382 factor:1 | 1 (-2.22146) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02285 HOMO: -6.54434 LUMO: 0.11157 factor:1 | 1 (-2.56612) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11256 HOMO: -6.53617 LUMO: 0.32926 factor:1 | 1 (-2.65583) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.64286 HOMO: -6.62597 LUMO: -0.60137 factor:1 | 1 (-3.18613) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.62762 HOMO: -6.60965 LUMO: -0.75376 factor:1 | 1 (-3.17089) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05558 HOMO: -6.29399 LUMO: 0.06803 factor:1 | 1 (-2.59885) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07869 HOMO: -6.60692 LUMO: -0.47076 factor:1 | 1 (-2.62195) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52033 HOMO: -7.33891 LUMO: 0.39184 factor:1 | 1 (-3.06359) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.19005 HOMO: -6.60692 LUMO: 1.46125 factor:1 | 1 (-3.73332) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.48707 HOMO: -6.21780 LUMO: 2.09256 factor:1 | 1 (-3.03034) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.56308 HOMO: -6.28311 LUMO: 1.80411 factor:1 | 1 (-3.10634) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.17185 HOMO: -6.51168 LUMO: 1.84765 factor:1 | 1 (-3.71512) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.04918 HOMO: -6.66951 LUMO: 2.01636 factor:1 | 1 (-3.59245) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55900 HOMO: -6.75387 LUMO: 1.73881 factor:1 | 1 (-2.10227) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13197 HOMO: -6.77291 LUMO: 1.89935 factor:1 | 1 (-2.67523) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10470 HOMO: -6.36474 LUMO: 1.61091 factor:1 | 1 (-2.64797) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06100 HOMO: -6.60420 LUMO: 1.40955 factor:1 | 1 (-2.60427) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50991 HOMO: -6.81645 LUMO: 1.59731 factor:1 | 1 (-2.05318) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07139 HOMO: -5.90215 LUMO: 2.12249 factor:1 | 1 (-2.61466) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54172 HOMO: -6.26950 LUMO: 1.62996 factor:1 | 1 (-2.08499) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.04960 HOMO: -6.41100 LUMO: 1.80684 factor:1 | 1 (-2.59286) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.86369 HOMO: -6.64230 LUMO: 2.23405 factor:1 | 1 (-2.40696) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11648 HOMO: -6.66951 LUMO: 2.21501 factor:1 | 1 (-2.65975) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45508 HOMO: -6.90897 LUMO: 2.00004 factor:1 | 1 (-1.99835) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.08380 HOMO: -6.61781 LUMO: 1.42043 factor:1 | 1 (-2.62707) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02679 HOMO: -6.56611 LUMO: 1.60003 factor:1 | 1 (-2.57006) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92627 HOMO: -6.70489 LUMO: 1.78779 factor:1 | 1 (-2.46954) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47625 HOMO: -6.46815 LUMO: 1.59459 factor:1 | 1 (-2.01952) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35143 HOMO: -6.31304 LUMO: 1.36873 factor:1 | 1 (-1.89470) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.21042 HOMO: -6.22597 LUMO: 1.54833 factor:1 | 1 (-2.75368) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.57801 HOMO: -5.63004 LUMO: 1.96466 factor:1 | 1 (-3.12128) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.37974 HOMO: -7.02598 LUMO: 1.79323 factor:1 | 1 (-3.92301) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.37958 HOMO: -6.78924 LUMO: 2.10888 factor:1 | 1 (-3.92285) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.38793 HOMO: -6.13345 LUMO: 2.07351 factor:1 | 1 (-3.93120) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06073 HOMO: -6.46270 LUMO: -0.37552 factor:1 | 1 (-2.60399) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99844 HOMO: -6.51985 LUMO: -0.49525 factor:1 | 1 (-2.54171) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65506 HOMO: -6.60965 LUMO: 1.90480 factor:1 | 1 (-2.19833) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44858 HOMO: -6.51168 LUMO: 1.92112 factor:1 | 1 (-1.99185) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17725 HOMO: -6.71305 LUMO: 1.91024 factor:1 | 1 (-1.72052) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06894 HOMO: -6.86815 LUMO: 2.02997 factor:1 | 1 (-2.61221) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.99446 HOMO: -6.69944 LUMO: 1.95106 factor:1 | 1 (-3.53773) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.04992 HOMO: -6.45182 LUMO: 1.66806 factor:1 | 1 (-2.59319) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.06962 HOMO: -6.44638 LUMO: 2.16058 factor:1 | 1 (-3.61288) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.98480 HOMO: -6.65591 LUMO: 1.95106 factor:1 | 1 (-3.52807) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.42789 HOMO: -6.35114 LUMO: 1.42316 factor:1 | 1 (-2.97116) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68814 HOMO: -6.48719 LUMO: 1.59187 factor:1 | 1 (-3.23141) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.34713 HOMO: -7.05591 LUMO: 1.61908 factor:1 | 1 (-2.89039) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.42472 HOMO: -6.92258 LUMO: 1.87214 factor:1 | 1 (-0.96799) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03771 HOMO: -5.85861 LUMO: 2.11705 factor:1 | 1 (-2.58097) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13088 HOMO: -6.27767 LUMO: 1.75513 factor:1 | 1 (-2.67414) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81523 HOMO: -6.16882 LUMO: 1.73881 factor:1 | 1 (-2.35849) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32801 HOMO: -6.62053 LUMO: 1.39594 factor:1 | 1 (-0.87128) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29926 HOMO: -5.46405 LUMO: 1.68166 factor:1 | 1 (-2.84253) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39894 HOMO: -6.39740 LUMO: 1.68711 factor:1 | 1 (-2.94220) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07025 HOMO: -6.99333 LUMO: 2.08439 factor:1 | 1 (-2.61352) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94582 HOMO: -6.16882 LUMO: 1.71976 factor:1 | 1 (-1.48909) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06520 HOMO: -7.19741 LUMO: 2.24766 factor:1 | 1 (-1.60847) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74008 HOMO: -6.77291 LUMO: 2.17691 factor:1 | 1 (-1.28334) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30678 HOMO: -6.29944 LUMO: 2.16603 factor:1 | 1 (-1.85005) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.67126 HOMO: -6.10079 LUMO: 1.83949 factor:1 | 1 (-1.21453) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.35280 HOMO: -6.63686 LUMO: 2.05990 factor:1 | 1 (-0.89607) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05504 HOMO: -6.91713 LUMO: 1.87486 factor:1 | 1 (-2.59831) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.61053 HOMO: -6.63958 LUMO: 1.79323 factor:1 | 1 (-3.15380) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10748 HOMO: -6.61781 LUMO: 1.70071 factor:1 | 1 (-2.65074) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76423 HOMO: -6.20420 LUMO: 1.82861 factor:1 | 1 (-2.30750) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55330 HOMO: -6.47903 LUMO: -2.16875 factor:1 | 1 (-1.09656) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.49230 HOMO: -6.53073 LUMO: 2.18235 factor:1 | 1 (-3.03557) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65282 HOMO: -7.01782 LUMO: 1.72520 factor:1 | 1 (-3.19609) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24244 HOMO: -6.66135 LUMO: -0.75648 factor:1 | 1 (-2.78571) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15268 HOMO: -7.56749 LUMO: 0.22585 factor:1 | 1 (-1.69595) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35293 HOMO: -6.45182 LUMO: -0.71294 factor:1 | 1 (-1.89620) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98397 HOMO: -6.31032 LUMO: -0.34286 factor:1 | 1 (-1.52724) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68306 HOMO: -6.41917 LUMO: 2.04085 factor:1 | 1 (-2.22633) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25768 HOMO: -6.61781 LUMO: 1.98915 factor:1 | 1 (-2.80095) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.45499 HOMO: -5.86405 LUMO: 1.57282 factor:1 | 1 (-2.99826) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.08448 HOMO: -6.44094 LUMO: 1.80956 factor:1 | 1 (-2.62775) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16880 HOMO: -6.59060 LUMO: 2.08167 factor:1 | 1 (-0.71207) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.62416 HOMO: -6.20147 LUMO: 1.69799 factor:1 | 1 (-1.16742) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45003 HOMO: -6.50352 LUMO: -0.41361 factor:1 | 1 (-0.99330) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.85411 HOMO: -6.10896 LUMO: -0.55783 factor:1 | 1 (-2.39738) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07681 HOMO: -6.74842 LUMO: -0.56872 factor:1 | 1 (-2.62008) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81631 HOMO: -6.59060 LUMO: -0.22041 factor:1 | 1 (-2.35958) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.03663 HOMO: -6.22052 LUMO: -0.60137 factor:1 | 1 (-0.57990) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19500 HOMO: -6.65863 LUMO: 0.07891 factor:1 | 1 (-0.73827) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11238 HOMO: -6.57427 LUMO: 1.71160 factor:1 | 1 (-1.65565) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.29979 HOMO: -5.84773 LUMO: 1.99459 factor:1 | 1 (-1.84305) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93028 HOMO: -6.02188 LUMO: 1.91296 factor:1 | 1 (-1.47355) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42235 HOMO: -6.17698 LUMO: 2.00004 factor:1 | 1 (-1.96561) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.46637 HOMO: -6.02732 LUMO: 1.90752 factor:1 | 1 (-0.00963) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.05767 HOMO: -6.68584 LUMO: -0.50885 factor:1 | 1 (-0.60094) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91318 HOMO: -6.61781 LUMO: -0.73471 factor:1 | 1 (-0.45644) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.23150 HOMO: -6.66407 LUMO: -0.79729 factor:1 | 1 (-0.77476) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30673 HOMO: -6.56339 LUMO: 0.23130 factor:1 | 1 (-1.84999) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.14056 HOMO: -6.76747 LUMO: 0.08980 factor:1 | -1 (0.31617) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.90485 HOMO: -6.70489 LUMO: -0.53334 factor:1 | 1 (-0.44812) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37099 HOMO: -7.28993 LUMO: 0.10885 factor:1 | 1 (-2.91426) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.54522 HOMO: -6.22052 LUMO: 0.51974 factor:1 | 1 (-3.08849) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.20625 HOMO: -6.81645 LUMO: 0.25307 factor:1 | 1 (-2.74952) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59751 HOMO: -6.80285 LUMO: 0.02721 factor:1 | 1 (-2.14077) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01099 HOMO: -6.51441 LUMO: 0.08163 factor:1 | 1 (-1.55426) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14792 HOMO: -6.73482 LUMO: -0.77008 factor:1 | 1 (-1.69119) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86274 HOMO: -6.29127 LUMO: -0.44355 factor:1 | 1 (-1.40601) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25772 HOMO: -6.72938 LUMO: -0.64763 factor:1 | 1 (-1.80099) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.03201 HOMO: -6.49264 LUMO: -0.74559 factor:1 | 1 (-0.57528) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.97563 HOMO: -6.67223 LUMO: -0.55239 factor:1 | 1 (-0.51889) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.22633 HOMO: -6.33481 LUMO: 0.33198 factor:1 | 1 (-2.76960) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33554 HOMO: -6.76475 LUMO: -0.25307 factor:1 | 1 (-1.87881) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39992 HOMO: -6.65318 LUMO: 0.03810 factor:1 | 1 (-2.94318) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46159 HOMO: -6.09263 LUMO: 0.21497 factor:1 | 1 (-2.00485) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10089 HOMO: -6.32120 LUMO: -0.85444 factor:1 | 1 (-2.64416) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18751 HOMO: -6.57155 LUMO: -0.67484 factor:1 | 1 (-1.73078) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.64349 HOMO: -6.53345 LUMO: -0.78913 factor:1 | 1 (-2.18676) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.34156 HOMO: -7.07768 LUMO: 0.28844 factor:1 | 1 (-1.88482) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10810 HOMO: -6.75114 LUMO: 0.18776 factor:1 | 1 (-2.65137) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.87647 HOMO: -6.77019 LUMO: -0.12245 factor:1 | 1 (-3.41974) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23091 HOMO: -6.43549 LUMO: 0.16327 factor:1 | 1 (-2.77417) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97920 HOMO: -6.69400 LUMO: -0.16327 factor:1 | 1 (-2.52247) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20281 HOMO: -6.38651 LUMO: -0.61770 factor:1 | 1 (-0.74608) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.03672 HOMO: -6.34297 LUMO: -0.33198 factor:1 | 1 (-0.57998) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.34833 HOMO: -7.51578 LUMO: 0.02177 factor:1 | 1 (-1.89160) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00824 HOMO: -6.47359 LUMO: -0.22585 factor:1 | 1 (-1.55151) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.72349 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-0.26675) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.86183 HOMO: -6.75659 LUMO: -0.57688 factor:1 | 1 (-0.40510) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33374 HOMO: -6.73754 LUMO: -0.61226 factor:1 | 1 (-2.87701) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07267 HOMO: -7.37429 LUMO: 0.31293 factor:1 | 1 (-2.61594) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37036 HOMO: -6.23413 LUMO: -0.90886 factor:1 | 1 (-2.91363) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.91688 HOMO: -6.51985 LUMO: -0.68028 factor:1 | 1 (-3.46015) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89904 HOMO: -6.52257 LUMO: -0.77280 factor:1 | 1 (-2.44230) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.13499 HOMO: -7.29537 LUMO: 0.31837 factor:1 | 1 (-2.67825) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73158 HOMO: -6.08447 LUMO: 0.25851 factor:1 | 1 (-2.27484) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10204 HOMO: -6.20964 LUMO: 0.13606 factor:1 | 1 (-1.64531) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88212 HOMO: -6.49808 LUMO: -0.14150 factor:1 | 1 (-1.42539) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93741 HOMO: -7.10761 LUMO: 0.28028 factor:1 | 1 (-1.48068) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.20558 HOMO: -6.60965 LUMO: -0.62858 factor:1 | 1 (-1.74885) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03282 HOMO: -6.40012 LUMO: -0.26939 factor:1 | 1 (-1.57608) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77001 HOMO: -6.65318 LUMO: -0.73199 factor:1 | 1 (-1.31328) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80114 HOMO: -6.51441 LUMO: -0.44899 factor:1 | 1 (-1.34441) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12433 HOMO: -6.28583 LUMO: -0.48708 factor:1 | 1 (-1.66760) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78881 HOMO: -6.96884 LUMO: 0.19864 factor:1 | 1 (-1.33208) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.69504 HOMO: -6.89809 LUMO: 0.34558 factor:1 | 1 (-1.23831) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02789 HOMO: -6.67495 LUMO: -0.15510 factor:1 | 1 (-1.57116) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90601 HOMO: -7.34980 LUMO: 0.19864 factor:1 | 1 (-1.44928) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.38239 HOMO: -6.71305 LUMO: -0.81634 factor:1 | 1 (-2.92566) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.12173 HOMO: -6.39468 LUMO: -0.47076 factor:1 | 1 (-3.66499) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18598 HOMO: -6.31304 LUMO: 1.39594 factor:1 | 1 (-2.72925) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.87199 HOMO: -6.57155 LUMO: 1.55105 factor:1 | 1 (-2.41526) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68464 HOMO: -6.68312 LUMO: 1.69255 factor:1 | 1 (-2.22791) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91944 HOMO: -6.61509 LUMO: 1.73881 factor:1 | 1 (-0.46270) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10888 HOMO: -6.17971 LUMO: 1.90208 factor:1 | 1 (-0.65215) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05801 HOMO: -6.53073 LUMO: 1.73337 factor:1 | 1 (-2.60127) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.84554 HOMO: -5.91303 LUMO: 1.90480 factor:1 | 1 (-2.38881) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.99451 HOMO: -6.42733 LUMO: 1.80139 factor:1 | 1 (-0.53778) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.11854 HOMO: -6.78924 LUMO: 2.31569 factor:1 | 1 (-0.66181) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.96888 HOMO: -6.04093 LUMO: 1.91568 factor:1 | 1 (-0.51215) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80683 HOMO: -6.90081 LUMO: 2.36739 factor:1 | 1 (-1.35009) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96079 HOMO: -6.60965 LUMO: 2.18507 factor:1 | 1 (-1.50405) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85243 HOMO: -6.75387 LUMO: 2.48712 factor:1 | 1 (-1.39570) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.40030 HOMO: -6.56883 LUMO: 1.71432 factor:1 | 1 (-2.94356) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.88844 HOMO: -6.41644 LUMO: 1.72792 factor:1 | 1 (-3.43171) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.04258 HOMO: -6.92530 LUMO: 2.54426 factor:1 | 1 (-2.58584) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.63416 HOMO: -6.41644 LUMO: 2.70209 factor:1 | 1 (-2.17743) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79069 HOMO: -6.29671 LUMO: 2.14698 factor:1 | 1 (-1.33396) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05736 HOMO: -6.29127 LUMO: 1.87486 factor:1 | 1 (-1.60063) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71506 HOMO: -6.75931 LUMO: 2.78917 factor:1 | 1 (-2.25833) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.66134 HOMO: -6.40828 LUMO: 1.86942 factor:1 | 1 (-3.20460) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74877 HOMO: -6.45726 LUMO: 1.97010 factor:1 | 1 (-2.29204) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.00562 HOMO: -6.43277 LUMO: 1.22723 factor:1 | 1 (-2.54889) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.54778 HOMO: -6.63414 LUMO: 1.62452 factor:1 | 1 (-3.09105) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83193 HOMO: -6.54162 LUMO: 2.16058 factor:1 | 1 (-2.37520) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79152 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-2.33479) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97218 HOMO: -6.20964 LUMO: 1.84221 factor:1 | 1 (-2.51545) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19140 HOMO: -6.58516 LUMO: 1.69799 factor:1 | 1 (-1.73467) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35192 HOMO: -6.44094 LUMO: 2.05446 factor:1 | 1 (-1.89519) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27606 HOMO: -6.61509 LUMO: 2.16058 factor:1 | 1 (-1.81933) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96805 HOMO: -6.65591 LUMO: 1.69527 factor:1 | 1 (-1.51132) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.63879 HOMO: -5.55112 LUMO: 1.80411 factor:1 | 1 (-2.18205) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73667 HOMO: -6.68312 LUMO: 2.38100 factor:1 | 1 (-2.27993) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.50237 HOMO: -6.51168 LUMO: 2.14698 factor:1 | 1 (-3.04563) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52520 HOMO: -6.04637 LUMO: 1.48302 factor:1 | 1 (-3.06846) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68986 HOMO: -6.81645 LUMO: -0.74287 factor:1 | 1 (-2.23313) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24946 HOMO: -6.96884 LUMO: -0.97961 factor:1 | 1 (-2.79273) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.43285 HOMO: -6.45998 LUMO: 0.09796 factor:1 | 1 (-1.97612) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22722 HOMO: -6.44638 LUMO: 0.09524 factor:1 | 1 (-0.77049) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32290 HOMO: -6.16338 LUMO: -0.54151 factor:1 | 1 (-0.86617) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.74735 HOMO: -6.35930 LUMO: -0.47892 factor:1 | 1 (-0.29062) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.95089 HOMO: -6.65318 LUMO: -0.00272 factor:1 | 1 (-0.49416) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.15899 HOMO: -6.50080 LUMO: 0.14694 factor:1 | -1 (0.29775) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.46275 HOMO: -6.60420 LUMO: 0.94968 factor:1 | 1 (-0.00601) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.58041 HOMO: -6.60148 LUMO: -0.77552 factor:1 | 1 (-0.12368) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12519.95817 HOMO: -6.81645 LUMO: -1.05580 factor:1 | -1 (0.49857) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.76474 HOMO: -6.57971 LUMO: -0.82178 factor:1 | 1 (-0.30801) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.69033 HOMO: -6.09263 LUMO: -0.45171 factor:1 | 1 (-1.23360) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52715 HOMO: -6.74298 LUMO: -0.61770 factor:1 | 1 (-1.07041) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22268 HOMO: -6.72393 LUMO: 1.21091 factor:1 | 1 (-0.76595) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.25642 HOMO: -6.30488 LUMO: 1.70071 factor:1 | 1 (-0.79969) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36867 HOMO: -6.38107 LUMO: 1.55649 factor:1 | 1 (-0.91194) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.06727 HOMO: -6.17154 LUMO: 1.46669 factor:1 | 1 (-0.61054) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.41313 HOMO: -6.86543 LUMO: 1.98643 factor:1 | 1 (-0.95640) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91459 HOMO: -6.69944 LUMO: 1.65173 factor:1 | 1 (-0.45786) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12621 HOMO: -6.77836 LUMO: 2.16331 factor:1 | 1 (-0.66948) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24186 HOMO: -6.42189 LUMO: 2.36467 factor:1 | 1 (-0.78513) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.04869 HOMO: -7.00965 LUMO: 2.04358 factor:1 | 1 (-0.59196) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.78368 HOMO: -6.36746 LUMO: 2.13881 factor:1 | 1 (-0.32694) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34143 HOMO: -6.37835 LUMO: 1.89935 factor:1 | 1 (-0.88470) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.65409 HOMO: -7.03959 LUMO: 1.27349 factor:1 | 1 (-1.19736) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.75327 HOMO: -6.67495 LUMO: -0.89253 factor:1 | 1 (-1.29654) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39299 HOMO: -6.71849 LUMO: -0.97961 factor:1 | 1 (-0.93626) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78699 HOMO: -6.47903 LUMO: 0.01633 factor:1 | 1 (-1.33026) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91513 HOMO: -6.38379 LUMO: 0.01088 factor:1 | 1 (-1.45839) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48183 HOMO: -6.49536 LUMO: -0.55239 factor:1 | 1 (-2.02510) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57239 HOMO: -6.53345 LUMO: -0.53879 factor:1 | 1 (-2.11566) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75835 HOMO: -6.16610 LUMO: 2.15514 factor:1 | 1 (-2.30162) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58996 HOMO: -6.35114 LUMO: 1.98643 factor:1 | 1 (-3.13323) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.53565 HOMO: -6.43277 LUMO: 2.16058 factor:1 | 1 (-3.07891) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69680 HOMO: -6.89809 LUMO: 2.20684 factor:1 | 1 (-2.24007) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41922 HOMO: -6.54434 LUMO: 1.93473 factor:1 | 1 (-1.96249) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53179 HOMO: -6.72938 LUMO: 2.03269 factor:1 | 1 (-2.07506) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75865 HOMO: -6.90353 LUMO: 2.19868 factor:1 | 1 (-2.30192) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73710 HOMO: -6.41372 LUMO: 2.02453 factor:1 | 1 (-2.28037) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61745 HOMO: -6.46543 LUMO: 1.90752 factor:1 | 1 (-2.16072) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30879 HOMO: -6.55522 LUMO: 2.11977 factor:1 | 1 (-1.85206) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53174 HOMO: -6.28855 LUMO: 2.02181 factor:1 | 1 (-2.07500) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.37905 HOMO: -6.45726 LUMO: 1.52112 factor:1 | 1 (-1.92232) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42733 HOMO: -6.37291 LUMO: 2.11705 factor:1 | 1 (-1.97059) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31301 HOMO: -6.88448 LUMO: 2.24494 factor:1 | 1 (-1.85628) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30907 HOMO: -6.86271 LUMO: 2.41637 factor:1 | 1 (-1.85233) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40817 HOMO: -6.69400 LUMO: 2.34562 factor:1 | 1 (-1.95144) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54755 HOMO: -6.18243 LUMO: 2.53882 factor:1 | 1 (-2.09081) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.20281 HOMO: -6.61237 LUMO: 2.54154 factor:1 | 1 (-1.74607) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34948 HOMO: -6.69672 LUMO: 2.16331 factor:1 | 1 (-0.89275) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12768 HOMO: -6.33481 LUMO: 2.34018 factor:1 | 1 (-0.67095) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12474 HOMO: -5.99739 LUMO: 2.37283 factor:1 | 1 (-0.66801) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83395 HOMO: -6.49808 LUMO: 2.47351 factor:1 | 1 (-2.37721) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58820 HOMO: -6.22052 LUMO: 1.86398 factor:1 | 1 (-2.13147) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28184 HOMO: -6.32665 LUMO: 2.28031 factor:1 | 1 (-0.82510) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26004 HOMO: -5.98378 LUMO: 2.16331 factor:1 | 1 (-0.80331) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.68183 HOMO: -6.08991 LUMO: 2.30208 factor:1 | 1 (-2.22510) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30994 HOMO: -7.07224 LUMO: 1.55105 factor:1 | 1 (-1.85320) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76053 HOMO: -6.84638 LUMO: 1.76874 factor:1 | 1 (-2.30380) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42861 HOMO: -6.68856 LUMO: 1.47758 factor:1 | 1 (-1.97187) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18885 HOMO: -6.69672 LUMO: 1.71976 factor:1 | 1 (-1.73211) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.50170 HOMO: -6.86543 LUMO: 2.24766 factor:1 | 1 (-1.04497) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36208 HOMO: -7.21646 LUMO: 1.71976 factor:1 | 1 (-0.90535) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.47719 HOMO: -6.94162 LUMO: 2.21773 factor:1 | 1 (-1.02045) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.14836 HOMO: -6.34842 LUMO: 2.04358 factor:1 | 1 (-0.69163) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.27950 HOMO: -6.53345 LUMO: 1.96738 factor:1 | 1 (-0.82276) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20603 HOMO: -6.34842 LUMO: 1.88303 factor:1 | 1 (-0.74929) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.41621 HOMO: -6.38651 LUMO: 2.08983 factor:1 | 1 (-0.95947) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.47961 HOMO: -6.01372 LUMO: 1.43676 factor:1 | 1 (-1.02288) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.72666 HOMO: -6.30216 LUMO: 1.41771 factor:1 | 1 (-1.26993) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01263 HOMO: -6.52801 LUMO: 1.77146 factor:1 | 1 (-1.55589) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25663 HOMO: -6.53617 LUMO: 1.72792 factor:1 | 1 (-1.79990) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33117 HOMO: -6.56611 LUMO: 2.20412 factor:1 | 1 (-0.87444) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39381 HOMO: -6.66679 LUMO: -0.72927 factor:1 | 1 (-0.93708) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.25571 HOMO: -6.85455 LUMO: -0.85444 factor:1 | 1 (-0.79898) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.52382 HOMO: -7.21646 LUMO: 0.27211 factor:1 | 1 (-2.06709) | 1 | 1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25768 HOMO: -6.57971 LUMO: -0.41361 factor:1 | 1 (-2.80095) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.11313 HOMO: -7.03142 LUMO: -1.14288 factor:1 | 1 (-3.65639) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.87350 HOMO: -6.29944 LUMO: 0.06803 factor:1 | 1 (-3.41677) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.45047 HOMO: -6.47359 LUMO: 0.28028 factor:1 | 1 (-3.99373) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.17819 HOMO: -6.42189 LUMO: 1.61364 factor:1 | 1 (-3.72146) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.99620 HOMO: -6.41100 LUMO: 1.80956 factor:1 | 1 (-3.53947) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30568 HOMO: -6.83278 LUMO: 1.83949 factor:1 | 1 (-2.84895) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.13141 HOMO: -6.78380 LUMO: -0.76192 factor:1 | 1 (-3.67468) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.64781 HOMO: -6.95795 LUMO: 2.13609 factor:1 | 1 (-3.19108) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39929 HOMO: -6.57155 LUMO: 1.89119 factor:1 | 1 (-2.94256) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36211 HOMO: -6.65591 LUMO: 1.93745 factor:1 | 1 (-0.90538) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34856 HOMO: -6.44638 LUMO: 2.26943 factor:1 | 1 (-0.89183) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33479 HOMO: -5.88038 LUMO: 1.90480 factor:1 | 1 (-0.87806) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99083 HOMO: -6.22052 LUMO: 2.17691 factor:1 | 1 (-1.53410) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26240 HOMO: -6.04637 LUMO: 2.23950 factor:1 | 1 (-1.80567) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24847 HOMO: -6.44366 LUMO: 2.24766 factor:1 | 1 (-1.79173) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85934 HOMO: -6.81917 LUMO: 2.08439 factor:1 | 1 (-1.40261) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36980 HOMO: -6.48447 LUMO: 2.28576 factor:1 | 1 (-1.91307) | -1 | -1 |
| G: -6256.09104 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06710 HOMO: -6.54434 LUMO: 1.99187 factor:1 | 1 (-1.61037) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91749 HOMO: -6.17698 LUMO: -0.65852 factor:1 | 1 (-1.46076) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22931 HOMO: -6.08174 LUMO: -0.58504 factor:1 | 1 (-1.77258) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85964 HOMO: -6.55250 LUMO: -0.86804 factor:1 | 1 (-1.40291) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.96638 HOMO: -6.57699 LUMO: -0.89525 factor:1 | 1 (-3.50964) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06084 HOMO: -6.63141 LUMO: -1.04220 factor:1 | 1 (-2.60410) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24315 HOMO: -6.69128 LUMO: -0.76736 factor:1 | 1 (-2.78642) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.99555 HOMO: -6.25318 LUMO: -1.03131 factor:1 | 1 (-3.53881) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.99911 HOMO: -6.69944 LUMO: 0.01905 factor:1 | 1 (-3.54238) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12503 HOMO: -6.28583 LUMO: 0.38368 factor:1 | 1 (-2.66829) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.64798 HOMO: -6.90081 LUMO: -0.83811 factor:1 | 1 (-3.19124) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72741 HOMO: -6.78380 LUMO: -0.10068 factor:1 | 1 (-2.27068) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18712 HOMO: -6.30488 LUMO: -0.98505 factor:1 | 1 (-2.73039) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.38773 HOMO: -6.29671 LUMO: -1.79051 factor:1 | 1 (-2.93099) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44825 HOMO: -6.76747 LUMO: -0.22041 factor:1 | 1 (-1.99152) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33481 HOMO: -6.22597 LUMO: -0.94968 factor:1 | 1 (-1.87808) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30591 HOMO: -6.73482 LUMO: 0.05987 factor:1 | 1 (-1.84918) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01121 HOMO: -6.28855 LUMO: 0.34831 factor:1 | 1 (-1.55448) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.52251 HOMO: -6.69400 LUMO: 0.25307 factor:1 | 1 (-2.06578) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10285 HOMO: -6.70216 LUMO: 0.61226 factor:1 | 1 (-2.64612) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32762 HOMO: -6.70216 LUMO: 0.17415 factor:1 | 1 (-1.87089) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10093 HOMO: -6.70761 LUMO: 0.24762 factor:1 | 1 (-1.64419) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33230 HOMO: -6.68856 LUMO: -0.84900 factor:1 | 1 (-1.87557) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12519.99125 HOMO: -6.71033 LUMO: -0.38640 factor:1 | -1 (0.46548) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12519.98821 HOMO: -6.24501 LUMO: -0.09252 factor:1 | -1 (0.46853) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.57839 HOMO: -6.81645 LUMO: -0.07347 factor:1 | 1 (-0.12166) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.86689 HOMO: -6.49536 LUMO: 0.09796 factor:1 | 1 (-0.41016) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.54065 HOMO: -6.71033 LUMO: -0.26395 factor:1 | 1 (-3.08392) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.35647 HOMO: -6.70489 LUMO: -0.09252 factor:1 | 1 (-1.89974) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57089 HOMO: -6.23685 LUMO: 0.39729 factor:1 | 1 (-2.11416) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16808 HOMO: -6.69400 LUMO: -0.05442 factor:1 | 1 (-1.71135) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00014 HOMO: -6.36202 LUMO: 0.09796 factor:1 | 1 (-1.54340) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19393 HOMO: -6.54978 LUMO: 0.15510 factor:1 | 1 (-1.73720) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.87835 HOMO: -6.77836 LUMO: 0.25851 factor:1 | 1 (-0.42161) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.04390 HOMO: -5.70623 LUMO: 0.73471 factor:1 | 1 (-0.58717) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.00278 HOMO: -5.58378 LUMO: 0.89253 factor:1 | 1 (-0.54605) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.29219 HOMO: -5.68718 LUMO: 0.87893 factor:1 | 1 (-2.83545) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53242 HOMO: -5.10486 LUMO: 1.11567 factor:1 | 1 (-2.07568) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03509 HOMO: -4.59328 LUMO: 1.27621 factor:1 | 1 (-2.57836) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22090 HOMO: -4.45450 LUMO: 1.82044 factor:1 | 1 (-1.76417) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56942 HOMO: -4.64226 LUMO: 1.70615 factor:1 | 1 (-2.11269) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32022 HOMO: -5.04227 LUMO: 1.04492 factor:1 | 1 (-1.86349) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33835 HOMO: -4.85723 LUMO: 0.93607 factor:1 | 1 (-1.88161) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32847 HOMO: -4.72934 LUMO: 1.00410 factor:1 | 1 (-1.87174) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46436 HOMO: -4.56335 LUMO: 1.56738 factor:1 | 1 (-2.00763) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13369 HOMO: -5.48854 LUMO: 0.33198 factor:1 | 1 (-1.67696) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11336 HOMO: -4.97424 LUMO: 1.33608 factor:1 | 1 (-1.65663) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26400 HOMO: -4.60145 LUMO: 1.74697 factor:1 | 1 (-1.80727) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01551 HOMO: -5.60010 LUMO: 0.74831 factor:1 | 1 (-1.55878) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14294 HOMO: -5.66541 LUMO: 0.66668 factor:1 | 1 (-1.68621) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33297 HOMO: -6.50080 LUMO: 0.07075 factor:1 | 1 (-0.87623) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.31362 HOMO: -5.79603 LUMO: 0.22313 factor:1 | 1 (-0.85689) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29944 HOMO: -4.68036 LUMO: 1.29798 factor:1 | 1 (-0.84271) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28584 HOMO: -4.84363 LUMO: 1.34424 factor:1 | 1 (-0.82910) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.25239 HOMO: -4.62321 LUMO: 1.82861 factor:1 | 1 (-0.79566) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10540 HOMO: -5.83684 LUMO: 0.82178 factor:1 | 1 (-0.64867) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61168 HOMO: -5.27629 LUMO: 0.57960 factor:1 | 1 (-2.15495) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60034 HOMO: -5.15928 LUMO: -2.96876 factor:1 | 1 (-2.14360) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24716 HOMO: -5.08853 LUMO: 0.89253 factor:1 | 1 (-1.79043) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29144 HOMO: -6.42461 LUMO: 0.04354 factor:1 | 1 (-0.83471) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.90425 HOMO: -6.42733 LUMO: -0.00544 factor:1 | 1 (-0.44752) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09919 HOMO: -5.87494 LUMO: 0.69933 factor:1 | 1 (-0.64246) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.17898 HOMO: -5.07492 LUMO: 1.02587 factor:1 | 1 (-0.72224) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69441 HOMO: -4.44362 LUMO: 1.99187 factor:1 | 1 (-2.23767) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27225 HOMO: -5.82052 LUMO: 0.43810 factor:1 | 1 (-1.81552) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71808 HOMO: -5.75793 LUMO: 0.76464 factor:1 | 1 (-2.26135) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84035 HOMO: -5.09669 LUMO: 0.72382 factor:1 | 1 (-1.38362) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07880 HOMO: -6.75387 LUMO: -2.02453 factor:1 | 1 (-1.62207) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57528 HOMO: -5.02322 LUMO: 1.14832 factor:1 | 1 (-2.11854) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77556 HOMO: -5.75521 LUMO: 0.73471 factor:1 | 1 (-1.31883) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15622 HOMO: -5.89943 LUMO: 0.54967 factor:1 | 1 (-1.69949) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96484 HOMO: -5.80147 LUMO: 0.72382 factor:1 | 1 (-1.50811) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80110 HOMO: -6.16066 LUMO: 0.39457 factor:1 | 1 (-2.34437) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57598 HOMO: -5.98650 LUMO: 0.76736 factor:1 | 1 (-2.11925) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26346 HOMO: -4.74839 LUMO: 1.88847 factor:1 | 1 (-1.80673) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07312 HOMO: -5.62459 LUMO: 0.26939 factor:1 | 1 (-1.61638) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.70291 HOMO: -4.88172 LUMO: 1.30070 factor:1 | 1 (-0.24618) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24352 HOMO: -5.09397 LUMO: 0.98505 factor:1 | 1 (-0.78679) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.90101 HOMO: -6.50080 LUMO: -0.28300 factor:1 | 1 (-0.44428) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18964 HOMO: -5.04227 LUMO: 1.49935 factor:1 | 1 (-1.73290) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10776 HOMO: -5.22731 LUMO: 0.88437 factor:1 | 1 (-1.65102) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25282 HOMO: -4.95519 LUMO: 1.25717 factor:1 | 1 (-1.79609) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14299 HOMO: -4.61233 LUMO: 1.27621 factor:1 | 1 (-1.68626) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95924 HOMO: -4.70757 LUMO: 1.63813 factor:1 | 1 (-1.50250) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32969 HOMO: -4.85179 LUMO: 1.11839 factor:1 | 1 (-1.87296) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.71090 HOMO: -4.97696 LUMO: 1.00138 factor:1 | 1 (-2.25416) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39152 HOMO: -5.64636 LUMO: 0.81090 factor:1 | 1 (-1.93478) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86285 HOMO: -4.37831 LUMO: 1.90208 factor:1 | 1 (-1.40612) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17864 HOMO: -4.67764 LUMO: 1.54561 factor:1 | 1 (-1.72191) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67092 HOMO: -5.87766 LUMO: 0.42994 factor:1 | 1 (-2.21419) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.85631 HOMO: -6.03821 LUMO: 0.32382 factor:1 | 1 (-2.39958) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91014 HOMO: -5.99739 LUMO: 0.69389 factor:1 | 1 (-2.45341) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.82777 HOMO: -6.43821 LUMO: 0.15238 factor:1 | 1 (-2.37104) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.48360 HOMO: -6.63414 LUMO: -0.07347 factor:1 | 1 (-2.02687) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.82774 HOMO: -6.50080 LUMO: 0.10068 factor:1 | 1 (-2.37101) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80586 HOMO: -6.49264 LUMO: 0.19592 factor:1 | 1 (-2.34913) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10880 HOMO: -5.83956 LUMO: 0.12517 factor:1 | 1 (-0.65207) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21830 HOMO: -6.50896 LUMO: 0.19048 factor:1 | 1 (-0.76157) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.83448 HOMO: -6.56611 LUMO: 0.04898 factor:1 | 1 (-0.37775) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38478 HOMO: -6.68040 LUMO: -0.08436 factor:1 | 1 (-0.92804) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91688 HOMO: -6.73754 LUMO: -0.08708 factor:1 | 1 (-0.46014) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.75040 HOMO: -6.80285 LUMO: -0.10612 factor:1 | 1 (-0.29367) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.96765 HOMO: -6.35658 LUMO: 0.02177 factor:1 | 1 (-0.51092) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78579 HOMO: -5.74160 LUMO: 0.14694 factor:1 | 1 (-1.32906) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16363 HOMO: -4.78376 LUMO: 0.92791 factor:1 | 1 (-0.70690) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15362 HOMO: -5.90215 LUMO: 0.36463 factor:1 | 1 (-0.69688) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39340 HOMO: -4.99329 LUMO: 0.85988 factor:1 | 1 (-0.93667) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84914 HOMO: -4.93887 LUMO: 1.33608 factor:1 | 1 (-1.39241) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.69807 HOMO: -5.19193 LUMO: 0.50341 factor:1 | 1 (-0.24134) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79423 HOMO: -6.64502 LUMO: -1.98643 factor:1 | 1 (-1.33749) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77575 HOMO: -5.15384 LUMO: 0.94968 factor:1 | 1 (-1.31902) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86163 HOMO: -6.31032 LUMO: 0.08436 factor:1 | 1 (-1.40490) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.57018 HOMO: -4.88716 LUMO: 0.82995 factor:1 | 1 (-0.11344) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.78409 HOMO: -5.57017 LUMO: 0.19320 factor:1 | 1 (-0.32735) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.64659 HOMO: -4.92254 LUMO: 0.93879 factor:1 | 1 (-0.18985) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.78956 HOMO: -4.77288 LUMO: 1.60003 factor:1 | 1 (-0.33282) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.57924 HOMO: -4.97696 LUMO: 0.89798 factor:1 | 1 (-0.12251) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48007 HOMO: -5.00690 LUMO: 1.14288 factor:1 | 1 (-1.02334) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.71986 HOMO: -4.88444 LUMO: 1.48574 factor:1 | 1 (-1.26313) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.68832 HOMO: -5.03955 LUMO: 1.51023 factor:1 | 1 (-1.23159) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80963 HOMO: -5.22459 LUMO: 0.99049 factor:1 | 1 (-1.35290) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52282 HOMO: -5.29534 LUMO: 0.96056 factor:1 | 1 (-1.06609) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24246 HOMO: -5.35520 LUMO: 0.68301 factor:1 | 1 (-0.78573) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13242 HOMO: -5.27357 LUMO: 1.18642 factor:1 | 1 (-0.67569) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39071 HOMO: -5.79875 LUMO: 0.61770 factor:1 | 1 (-0.93398) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.47515 HOMO: -7.64640 LUMO: -2.45175 factor:1 | 1 (-1.01841) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13343 HOMO: -7.46953 LUMO: -1.29798 factor:1 | 1 (-0.67669) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34649 HOMO: -7.95389 LUMO: -0.37280 factor:1 | 1 (-0.88976) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91880 HOMO: -7.23279 LUMO: -1.19186 factor:1 | 1 (-1.46207) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17004 HOMO: -7.14299 LUMO: -1.12927 factor:1 | 1 (-1.71331) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.70247 HOMO: -6.93074 LUMO: 0.31565 factor:1 | 1 (-1.24574) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93322 HOMO: -6.63141 LUMO: 0.28028 factor:1 | 1 (-1.47649) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94160 HOMO: -7.10489 LUMO: -1.07213 factor:1 | 1 (-1.48487) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.76896 HOMO: -7.00693 LUMO: -0.69389 factor:1 | 1 (-0.31222) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.98725 HOMO: -8.50356 LUMO: -1.79595 factor:1 | 1 (-0.53051) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36067 HOMO: -7.79334 LUMO: -2.33746 factor:1 | 1 (-0.90394) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43354 HOMO: -7.24367 LUMO: -0.85172 factor:1 | 1 (-0.97681) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43852 HOMO: -7.94028 LUMO: -0.20136 factor:1 | 1 (-0.98179) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38987 HOMO: -7.22462 LUMO: 0.84627 factor:1 | 1 (-0.93313) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57327 HOMO: -6.54978 LUMO: 0.34831 factor:1 | 1 (-1.11654) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22633 HOMO: -6.86815 LUMO: 0.32109 factor:1 | 1 (-0.76959) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44930 HOMO: -7.17564 LUMO: -1.28438 factor:1 | 1 (-0.99256) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13625 HOMO: -7.03142 LUMO: -1.12655 factor:1 | 1 (-1.67951) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87992 HOMO: -7.39878 LUMO: 0.15783 factor:1 | 1 (-1.42318) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27954 HOMO: -7.25728 LUMO: 0.42178 factor:1 | 1 (-1.82281) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04751 HOMO: -6.86543 LUMO: 0.93879 factor:1 | 1 (-1.59078) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.37865 HOMO: -7.09673 LUMO: -0.69661 factor:1 | 1 (-1.92191) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.40431 HOMO: -7.74708 LUMO: 0.01088 factor:1 | 1 (-0.94758) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13532 HOMO: -6.80557 LUMO: 0.46531 factor:1 | 1 (-1.67859) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55790 HOMO: -7.29265 LUMO: 1.31975 factor:1 | 1 (-1.10116) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82321 HOMO: -6.93618 LUMO: 0.29388 factor:1 | 1 (-1.36647) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30137 HOMO: -6.53073 LUMO: 0.71022 factor:1 | 1 (-1.84463) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57545 HOMO: -6.41917 LUMO: -1.24084 factor:1 | 1 (-1.11871) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80040 HOMO: -6.67495 LUMO: -1.09118 factor:1 | 1 (-1.34367) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.60731 HOMO: -6.97156 LUMO: -0.53606 factor:1 | 1 (-1.15058) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83167 HOMO: -6.85183 LUMO: -0.45715 factor:1 | 1 (-1.37494) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06465 HOMO: -7.12666 LUMO: -0.67484 factor:1 | 1 (-1.60792) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02860 HOMO: -7.49946 LUMO: -0.14694 factor:1 | 1 (-1.57187) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22449 HOMO: -7.44231 LUMO: 0.58232 factor:1 | 1 (-1.76776) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27791 HOMO: -7.36340 LUMO: -0.68301 factor:1 | 1 (-1.82118) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.64649 HOMO: -6.13073 LUMO: -0.54967 factor:1 | 1 (-2.18975) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78986 HOMO: -7.81511 LUMO: -0.06531 factor:1 | 1 (-2.33313) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75827 HOMO: -7.26816 LUMO: -1.02587 factor:1 | 1 (-2.30154) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50164 HOMO: -7.98110 LUMO: -0.17960 factor:1 | 1 (-2.04491) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42621 HOMO: -7.44776 LUMO: -1.00954 factor:1 | 1 (-1.96948) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12842 HOMO: -7.47769 LUMO: -1.02859 factor:1 | 1 (-0.67169) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13451 HOMO: -6.75659 LUMO: 0.39457 factor:1 | 1 (-0.67778) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12891 HOMO: -6.71849 LUMO: 0.36735 factor:1 | 1 (-0.67218) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09672 HOMO: -7.64096 LUMO: -1.43948 factor:1 | 1 (-0.63998) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09557 HOMO: -7.83144 LUMO: -1.36601 factor:1 | 1 (-0.63884) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.82395 HOMO: -7.19469 LUMO: 0.35103 factor:1 | 1 (-0.36722) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29133 HOMO: -7.03414 LUMO: 0.20409 factor:1 | 1 (-0.83460) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.41155 HOMO: -7.22734 LUMO: 0.31293 factor:1 | 1 (-0.95482) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48810 HOMO: -6.93618 LUMO: 0.56055 factor:1 | 1 (-1.03137) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38206 HOMO: -6.94707 LUMO: -0.88709 factor:1 | 1 (-0.92532) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.95013 HOMO: -6.86543 LUMO: -0.83267 factor:1 | 1 (-0.49340) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37615 HOMO: -6.82189 LUMO: -1.15376 factor:1 | 1 (-0.91942) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30322 HOMO: -6.65046 LUMO: -0.46531 factor:1 | 1 (-0.84649) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.08004 HOMO: -6.52529 LUMO: 0.20953 factor:1 | 1 (-0.62330) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.99448 HOMO: -6.80557 LUMO: 0.44355 factor:1 | 1 (-0.53775) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.64174 HOMO: -6.93074 LUMO: -0.81634 factor:1 | 1 (-0.18501) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38494 HOMO: -7.43143 LUMO: -0.45987 factor:1 | 1 (-0.92821) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.07364 HOMO: -7.07224 LUMO: -0.68028 factor:1 | 1 (-0.61691) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.24091 HOMO: -6.68040 LUMO: -0.71566 factor:1 | 1 (-0.78418) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.43403 HOMO: -6.26406 LUMO: -1.09934 factor:1 | 1 (-0.97730) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.66144 HOMO: -5.94569 LUMO: -0.72110 factor:1 | 1 (-1.20470) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16610 HOMO: -6.12256 LUMO: -0.42178 factor:1 | 1 (-1.70936) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10242 HOMO: -6.09807 LUMO: 0.11429 factor:1 | 1 (-1.64569) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11293 HOMO: -7.35252 LUMO: -0.55783 factor:1 | 1 (-1.65619) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.76734 HOMO: -7.57837 LUMO: -0.76736 factor:1 | 1 (-1.31061) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90438 HOMO: -6.16066 LUMO: 0.01905 factor:1 | 1 (-1.44765) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83140 HOMO: -6.13345 LUMO: -0.41906 factor:1 | 1 (-1.37466) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77567 HOMO: -6.10351 LUMO: -0.33742 factor:1 | 1 (-1.31894) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.54625 HOMO: -7.24639 LUMO: -0.51702 factor:1 | 1 (-1.08952) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.64500 HOMO: -6.98244 LUMO: -1.82044 factor:1 | 1 (-1.18827) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.81880 HOMO: -6.37563 LUMO: -1.67622 factor:1 | 1 (-1.36207) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93611 HOMO: -5.79058 LUMO: -2.55243 factor:1 | 1 (-1.47937) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87099 HOMO: -6.34025 LUMO: -0.27483 factor:1 | 1 (-1.41426) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28226 HOMO: -6.05453 LUMO: -0.51157 factor:1 | 1 (-1.82553) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59685 HOMO: -7.53755 LUMO: -0.38912 factor:1 | 1 (-2.14012) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.49753 HOMO: -7.00421 LUMO: -0.50885 factor:1 | 1 (-2.04080) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28264 HOMO: -7.52123 LUMO: -0.37552 factor:1 | 1 (-1.82591) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59933 HOMO: -6.70489 LUMO: -1.04764 factor:1 | 1 (-2.14260) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39603 HOMO: -7.06408 LUMO: -1.16737 factor:1 | 1 (-1.93930) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08694 HOMO: -6.71849 LUMO: -1.02315 factor:1 | 1 (-1.63021) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.57189 HOMO: -6.16610 LUMO: -0.50885 factor:1 | 1 (-3.11516) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69528 HOMO: -6.48447 LUMO: 0.07619 factor:1 | 1 (-2.23854) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44295 HOMO: -7.06135 LUMO: 0.09796 factor:1 | 1 (-1.98621) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30410 HOMO: -6.47359 LUMO: 0.22585 factor:1 | 1 (-2.84737) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60521 HOMO: -6.10896 LUMO: -0.62314 factor:1 | 1 (-2.14847) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58257 HOMO: -6.88176 LUMO: -0.96600 factor:1 | 1 (-2.12584) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38539 HOMO: -6.67495 LUMO: 0.21769 factor:1 | 1 (-1.92866) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.56417 HOMO: -6.84911 LUMO: 0.38368 factor:1 | 1 (-2.10744) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58934 HOMO: -6.83550 LUMO: 1.29798 factor:1 | 1 (-2.13261) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69413 HOMO: -6.67495 LUMO: 1.46941 factor:1 | 1 (-2.23740) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28523 HOMO: -6.81917 LUMO: 1.30887 factor:1 | 1 (-1.82850) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39241 HOMO: -6.56611 LUMO: 0.66396 factor:1 | 1 (-1.93568) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30256 HOMO: -6.76203 LUMO: 0.60137 factor:1 | 1 (-1.84583) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46583 HOMO: -6.55794 LUMO: 0.34286 factor:1 | 1 (-2.00910) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41018 HOMO: -6.83550 LUMO: 0.35919 factor:1 | 1 (-1.95345) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17611 HOMO: -7.17836 LUMO: 0.63130 factor:1 | 1 (-1.71938) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14789 HOMO: -6.29944 LUMO: -0.69389 factor:1 | 1 (-1.69116) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.81581 HOMO: -7.06680 LUMO: -0.95784 factor:1 | 1 (-0.35908) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.72553 HOMO: -6.84638 LUMO: -0.87076 factor:1 | 1 (-0.26879) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12842 HOMO: -6.96339 LUMO: -1.05308 factor:1 | 1 (-0.67169) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.01106 HOMO: -6.75387 LUMO: -1.04220 factor:1 | 1 (-0.55432) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.64194 HOMO: -6.71849 LUMO: -0.84355 factor:1 | 1 (-2.18521) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31394 HOMO: -7.16748 LUMO: 0.51702 factor:1 | 1 (-1.85720) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.72142 HOMO: -6.92530 LUMO: 0.71566 factor:1 | 1 (-0.26469) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.03982 HOMO: -7.11034 LUMO: 0.01905 factor:1 | 1 (-0.58309) | 1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59707 HOMO: -6.79468 LUMO: 0.77008 factor:1 | 1 (-2.14034) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.60611 HOMO: -6.52801 LUMO: 0.98233 factor:1 | 1 (-2.14937) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31415 HOMO: -6.76475 LUMO: 0.53334 factor:1 | 1 (-1.85742) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80106 HOMO: -5.29261 LUMO: 0.57416 factor:1 | 1 (-1.34432) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04800 HOMO: -6.57971 LUMO: 0.12789 factor:1 | 1 (-1.59127) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38154 HOMO: -6.99333 LUMO: 0.51430 factor:1 | 1 (-0.92481) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22290 HOMO: -6.41917 LUMO: 0.19048 factor:1 | 1 (-0.76616) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26619 HOMO: -6.16066 LUMO: 1.77146 factor:1 | 1 (-0.80946) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.31169 HOMO: -6.90353 LUMO: 1.65717 factor:1 | 1 (-0.85495) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.97179 HOMO: -5.94569 LUMO: 1.29526 factor:1 | 1 (-0.51506) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.08839 HOMO: -6.60420 LUMO: 1.33880 factor:1 | 1 (-0.63166) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.23130 HOMO: -6.23957 LUMO: 0.09524 factor:1 | 1 (-0.77457) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26377 HOMO: -6.80013 LUMO: 1.34696 factor:1 | 1 (-0.80704) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30820 HOMO: -7.53483 LUMO: -1.52384 factor:1 | 1 (-1.85146) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40931 HOMO: -7.62463 LUMO: -1.65717 factor:1 | 1 (-1.95258) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19854 HOMO: -7.62463 LUMO: -1.61364 factor:1 | 1 (-0.74181) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.35161 HOMO: -8.04096 LUMO: -1.66806 factor:1 | 1 (-0.89487) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06871 HOMO: -7.18381 LUMO: -1.17553 factor:1 | 1 (-1.61198) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04452 HOMO: -7.69538 LUMO: -1.36601 factor:1 | 1 (-1.58778) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07567 HOMO: -7.95117 LUMO: -1.48302 factor:1 | 1 (-1.61894) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23423 HOMO: -6.98516 LUMO: 0.35919 factor:1 | 1 (-1.77750) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.89606 HOMO: -7.91579 LUMO: -0.32109 factor:1 | 1 (-3.43933) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11518 HOMO: -6.75659 LUMO: -0.03537 factor:1 | 1 (-2.65844) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.88746 HOMO: -7.78518 LUMO: -2.36467 factor:1 | 1 (-3.43073) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.58035 HOMO: -7.96477 LUMO: -2.75651 factor:1 | 1 (-3.12362) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.77128 HOMO: -7.60286 LUMO: -2.35106 factor:1 | 1 (-2.31455) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02312 HOMO: -7.38245 LUMO: -1.21635 factor:1 | 1 (-2.56639) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.35826 HOMO: -7.91579 LUMO: -1.50479 factor:1 | 1 (-2.90152) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30741 HOMO: -8.07362 LUMO: -0.28028 factor:1 | 1 (-1.85067) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08291 HOMO: -7.38245 LUMO: -1.15921 factor:1 | 1 (-1.62618) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85461 HOMO: -7.18653 LUMO: -0.94968 factor:1 | 1 (-1.39788) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55727 HOMO: -6.88448 LUMO: 0.38096 factor:1 | 1 (-1.10054) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02626 HOMO: -6.97972 LUMO: 0.43266 factor:1 | 1 (-1.56953) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.85138 HOMO: -6.88992 LUMO: -0.43538 factor:1 | 1 (-0.39465) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.88790 HOMO: -7.97021 LUMO: -0.17143 factor:1 | 1 (-0.43116) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19171 HOMO: -6.92530 LUMO: 0.77280 factor:1 | 1 (-0.73498) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.07617 HOMO: -7.89674 LUMO: -0.09796 factor:1 | 1 (-0.61944) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.86537 HOMO: -7.02870 LUMO: 0.88709 factor:1 | 1 (-0.40863) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21824 HOMO: -6.78380 LUMO: 0.22041 factor:1 | 1 (-0.76151) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.58871 HOMO: -7.24911 LUMO: -0.82178 factor:1 | 1 (-0.13198) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.44783 HOMO: -6.77019 LUMO: 0.52790 factor:1 | -1 (0.00890) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.18450 HOMO: -8.56070 LUMO: -1.83405 factor:1 | 1 (-0.72777) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34480 HOMO: -7.74164 LUMO: -2.36195 factor:1 | 1 (-0.88807) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15830 HOMO: -7.39878 LUMO: -2.41637 factor:1 | 1 (-0.70156) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22714 HOMO: -7.61647 LUMO: -2.34018 factor:1 | 1 (-0.77041) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.06975 HOMO: -6.93346 LUMO: -0.57688 factor:1 | 1 (-0.61302) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.14504 HOMO: -6.85183 LUMO: -1.00410 factor:1 | 1 (-0.68831) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.00194 HOMO: -7.18925 LUMO: -1.12655 factor:1 | 1 (-0.54521) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16994 HOMO: -6.85183 LUMO: -1.60275 factor:1 | 1 (-0.71321) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.84000 HOMO: -7.51578 LUMO: 0.12517 factor:1 | 1 (-0.38327) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22940 HOMO: -7.36068 LUMO: 0.05714 factor:1 | 1 (-0.77267) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87594 HOMO: -7.49674 LUMO: 0.18776 factor:1 | 1 (-1.41921) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.52913 HOMO: -7.09401 LUMO: -1.24900 factor:1 | 1 (-1.07240) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46840 HOMO: -7.22462 LUMO: -1.61364 factor:1 | 1 (-1.01166) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.70008 HOMO: -7.74436 LUMO: -0.18776 factor:1 | 1 (-1.24334) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.67206 HOMO: -7.35252 LUMO: 0.75376 factor:1 | 1 (-0.21532) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.81837 HOMO: -7.75252 LUMO: 0.00816 factor:1 | 1 (-0.36164) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.58835 HOMO: -7.06680 LUMO: 0.24490 factor:1 | 1 (-0.13162) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.71219 HOMO: -7.49129 LUMO: 0.14150 factor:1 | 1 (-0.25546) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.34840 HOMO: -6.90625 LUMO: -1.11295 factor:1 | -1 (0.10833) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.79644 HOMO: -6.78380 LUMO: -0.93063 factor:1 | 1 (-0.33971) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.41063 HOMO: -7.79878 LUMO: 0.30477 factor:1 | 1 (-0.95390) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45985 HOMO: -7.87498 LUMO: 0.61770 factor:1 | 1 (-1.00312) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.22299 HOMO: -7.23823 LUMO: 0.30205 factor:1 | -1 (0.23375) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.26223 HOMO: -7.67633 LUMO: 0.13061 factor:1 | -1 (0.19451) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55009 HOMO: -7.79606 LUMO: 0.34558 factor:1 | 1 (-1.09335) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48652 HOMO: -6.66135 LUMO: -2.60141 factor:1 | 1 (-1.02979) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.23831 HOMO: -7.03142 LUMO: 0.50885 factor:1 | -1 (0.21843) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.17224 HOMO: -7.05591 LUMO: -0.06531 factor:1 | -1 (0.28450) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12519.76121 HOMO: -7.45592 LUMO: -1.39594 factor:1 | -1 (0.69552) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12519.74943 HOMO: -7.22462 LUMO: -1.10478 factor:1 | -1 (0.70731) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12519.98584 HOMO: -8.14709 LUMO: -0.55783 factor:1 | -1 (0.47089) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36091 HOMO: -7.22190 LUMO: -1.14560 factor:1 | 1 (-0.90418) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46875 HOMO: -7.28721 LUMO: -1.14016 factor:1 | 1 (-1.01202) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57346 HOMO: -6.97156 LUMO: 0.51702 factor:1 | 1 (-1.11673) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58103 HOMO: -7.37156 LUMO: 0.29388 factor:1 | 1 (-1.12429) | 1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39675 HOMO: -7.66273 LUMO: -1.59731 factor:1 | 1 (-0.94002) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22173 HOMO: -7.50490 LUMO: -1.49935 factor:1 | 1 (-0.76499) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26886 HOMO: -7.61102 LUMO: -1.45581 factor:1 | 1 (-0.81212) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32771 HOMO: -7.58653 LUMO: -1.61091 factor:1 | 1 (-0.87098) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19694 HOMO: -7.36068 LUMO: -1.14560 factor:1 | 1 (-0.74020) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.04793 HOMO: -6.96339 LUMO: 0.26939 factor:1 | 1 (-0.59119) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.87606 HOMO: -6.53617 LUMO: 0.22313 factor:1 | 1 (-0.41933) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.52231 HOMO: -7.33619 LUMO: -1.02587 factor:1 | 1 (-0.06558) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.96232 HOMO: -6.87904 LUMO: 0.33742 factor:1 | 1 (-0.50559) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92920 HOMO: -6.88448 LUMO: 0.58777 factor:1 | 1 (-1.47246) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24115 HOMO: -6.55522 LUMO: -1.51295 factor:1 | 1 (-1.78441) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44921 HOMO: -7.43415 LUMO: 0.10612 factor:1 | 1 (-0.99248) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.72715 HOMO: -7.54300 LUMO: -0.02449 factor:1 | 1 (-1.27042) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.59663 HOMO: -7.42054 LUMO: 0.28028 factor:1 | 1 (-0.13989) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.65255 HOMO: -6.98244 LUMO: -0.95784 factor:1 | 1 (-0.19581) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.55924 HOMO: -6.96884 LUMO: -1.12383 factor:1 | 1 (-0.10251) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.36843 HOMO: -6.80829 LUMO: -0.98233 factor:1 | -1 (0.08830) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.93723 HOMO: -7.60830 LUMO: 0.58504 factor:1 | 1 (-0.48050) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.82890 HOMO: -7.52123 LUMO: 0.08163 factor:1 | 1 (-0.37217) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28263 HOMO: -7.59742 LUMO: 0.00272 factor:1 | 1 (-0.82589) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37245 HOMO: -6.99333 LUMO: -1.33880 factor:1 | 1 (-0.91572) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98441 HOMO: -6.63958 LUMO: -1.39322 factor:1 | 1 (-1.52767) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24923 HOMO: -7.86137 LUMO: 0.01633 factor:1 | 1 (-1.79250) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19440 HOMO: -7.29537 LUMO: 0.14694 factor:1 | 1 (-1.73766) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41198 HOMO: -6.95523 LUMO: 0.48708 factor:1 | 1 (-1.95525) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.81047 HOMO: -7.10217 LUMO: -1.10478 factor:1 | 1 (-1.35374) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.58247 HOMO: -6.88176 LUMO: -0.96328 factor:1 | 1 (-1.12574) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53185 HOMO: -7.89130 LUMO: -0.13334 factor:1 | 1 (-1.07512) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46959 HOMO: -7.75252 LUMO: 0.25579 factor:1 | 1 (-1.01286) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82887 HOMO: -6.87632 LUMO: -0.93063 factor:1 | 1 (-1.37213) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74184 HOMO: -6.78108 LUMO: -0.86804 factor:1 | 1 (-1.28511) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.45104 HOMO: -5.98106 LUMO: 0.10340 factor:1 | 1 (-0.99430) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10738 HOMO: -6.40284 LUMO: -0.87349 factor:1 | 1 (-0.65065) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78345 HOMO: -6.77019 LUMO: -1.20819 factor:1 | 1 (-1.32672) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.42434 HOMO: -6.90081 LUMO: -1.00682 factor:1 | 1 (-0.96761) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27369 HOMO: -6.59060 LUMO: -0.26667 factor:1 | 1 (-1.81696) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45916 HOMO: -6.50896 LUMO: -0.48708 factor:1 | 1 (-2.00243) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.45233 HOMO: -6.20420 LUMO: -0.73471 factor:1 | 1 (-2.99559) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61068 HOMO: -6.17154 LUMO: -0.68573 factor:1 | 1 (-2.15394) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.54016 HOMO: -6.21236 LUMO: 0.09796 factor:1 | 1 (-3.08343) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47974 HOMO: -6.38379 LUMO: 0.58232 factor:1 | 1 (-2.02300) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37858 HOMO: -7.42871 LUMO: 0.40273 factor:1 | 1 (-2.92185) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.39815 HOMO: -6.54978 LUMO: 0.26395 factor:1 | 1 (-2.94141) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12405 HOMO: -7.14027 LUMO: 0.14150 factor:1 | 1 (-2.66731) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19010 HOMO: -7.25456 LUMO: -0.15783 factor:1 | 1 (-1.73337) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30822 HOMO: -6.90897 LUMO: 0.63403 factor:1 | 1 (-1.85149) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88647 HOMO: -6.49264 LUMO: 0.71022 factor:1 | 1 (-1.42974) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.44401 HOMO: -6.56067 LUMO: -1.03947 factor:1 | 1 (-1.98727) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.93195 HOMO: -6.79196 LUMO: -1.12655 factor:1 | 1 (-3.47522) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.89900 HOMO: -6.95251 LUMO: -1.09118 factor:1 | 1 (-3.44227) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.98254 HOMO: -7.47225 LUMO: -0.22041 factor:1 | 1 (-3.52581) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.44698 HOMO: -7.13483 LUMO: -0.98505 factor:1 | 1 (-3.99025) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15485 HOMO: -6.99061 LUMO: -1.05852 factor:1 | 1 (-2.69812) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.74330 HOMO: -6.52257 LUMO: -1.11022 factor:1 | 1 (-3.28656) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.03043 HOMO: -6.75114 LUMO: -1.09934 factor:1 | 1 (-3.57370) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25072 HOMO: -6.82189 LUMO: -0.89253 factor:1 | 1 (-2.79398) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72581 HOMO: -6.83278 LUMO: -0.97961 factor:1 | 1 (-2.26908) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67762 HOMO: -6.65318 LUMO: -0.84355 factor:1 | 1 (-2.22088) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39013 HOMO: -6.75931 LUMO: -0.88437 factor:1 | 1 (-1.93340) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40376 HOMO: -6.19059 LUMO: -0.45715 factor:1 | 1 (-1.94703) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.29108 HOMO: -7.09673 LUMO: -2.01908 factor:1 | 1 (-1.83435) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.43516 HOMO: -7.88042 LUMO: 0.38640 factor:1 | 1 (-1.97843) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.04883 HOMO: -7.83144 LUMO: 0.14422 factor:1 | 1 (-3.59209) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25368 HOMO: -7.46408 LUMO: 0.44627 factor:1 | 1 (-2.79695) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.07400 HOMO: -7.12394 LUMO: -2.04902 factor:1 | 1 (-3.61726) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.18385 HOMO: -6.78380 LUMO: -1.11295 factor:1 | 1 (-3.72712) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33308 HOMO: -7.12938 LUMO: -0.23674 factor:1 | 1 (-2.87635) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.02298 HOMO: -6.14705 LUMO: -0.20409 factor:1 | 1 (-3.56624) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07460 HOMO: -6.50080 LUMO: -0.28300 factor:1 | 1 (-2.61787) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27254 HOMO: -6.50352 LUMO: -0.62042 factor:1 | 1 (-2.81581) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37452 HOMO: -6.46543 LUMO: -0.53879 factor:1 | 1 (-0.91779) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16730 HOMO: -7.32803 LUMO: -0.52790 factor:1 | 1 (-0.71057) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30456 HOMO: -5.94025 LUMO: -0.17687 factor:1 | 1 (-0.84783) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19543 HOMO: -5.62187 LUMO: 0.05714 factor:1 | 1 (-1.73870) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98688 HOMO: -7.03414 LUMO: -1.04492 factor:1 | 1 (-1.53015) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25317 HOMO: -6.75387 LUMO: -2.02181 factor:1 | 1 (-1.79644) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11018 HOMO: -6.55250 LUMO: -0.75648 factor:1 | 1 (-1.65345) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85153 HOMO: -6.81101 LUMO: -1.02043 factor:1 | 1 (-1.39480) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97635 HOMO: -6.69672 LUMO: -2.81910 factor:1 | 1 (-1.51962) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07845 HOMO: -6.69128 LUMO: -2.58236 factor:1 | 1 (-1.62172) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.22100 HOMO: -6.73482 LUMO: -2.06807 factor:1 | 1 (-2.76427) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.12845 HOMO: -7.66545 LUMO: 0.17143 factor:1 | 1 (-3.67171) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.18613 HOMO: -6.87904 LUMO: -1.25172 factor:1 | 1 (-3.72940) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.70961 HOMO: -6.84366 LUMO: -0.19320 factor:1 | 1 (-3.25288) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96208 HOMO: -6.97972 LUMO: -0.97961 factor:1 | 1 (-2.50535) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15469 HOMO: -6.72121 LUMO: -0.70477 factor:1 | 1 (-2.69795) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.34944 HOMO: -7.18925 LUMO: 0.40001 factor:1 | 1 (-2.89271) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57389 HOMO: -6.72121 LUMO: 0.19592 factor:1 | 1 (-2.11715) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28907 HOMO: -6.85999 LUMO: -0.39457 factor:1 | 1 (-0.83234) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11597 HOMO: -6.90625 LUMO: 0.05987 factor:1 | 1 (-1.65924) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33824 HOMO: -7.00421 LUMO: 0.37552 factor:1 | 1 (-1.88150) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92623 HOMO: -6.56883 LUMO: -0.97689 factor:1 | 1 (-1.46950) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26936 HOMO: -6.66679 LUMO: 0.56055 factor:1 | 1 (-1.81263) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54926 HOMO: -6.75931 LUMO: 0.32926 factor:1 | 1 (-2.09253) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28270 HOMO: -6.53617 LUMO: -1.06397 factor:1 | 1 (-1.82597) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93959 HOMO: -6.78108 LUMO: 0.42722 factor:1 | 1 (-1.48286) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58608 HOMO: -7.05319 LUMO: 0.61498 factor:1 | 1 (-2.12935) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38948 HOMO: -6.78380 LUMO: 1.49391 factor:1 | 1 (-1.93274) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38616 HOMO: -7.21102 LUMO: 0.27211 factor:1 | 1 (-1.92942) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61239 HOMO: -6.67223 LUMO: 0.81362 factor:1 | 1 (-2.15566) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75329 HOMO: -6.69944 LUMO: 1.40683 factor:1 | 1 (-2.29656) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26011 HOMO: -7.02598 LUMO: 1.46941 factor:1 | 1 (-1.80338) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.51138 HOMO: -5.85045 LUMO: -0.76736 factor:1 | 1 (-2.05465) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.52638 HOMO: -6.53890 LUMO: -0.50885 factor:1 | 1 (-2.06964) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.43054 HOMO: -6.42733 LUMO: -0.63947 factor:1 | 1 (-1.97381) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.28116 HOMO: -6.82189 LUMO: -0.85444 factor:1 | 1 (-0.82442) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.93492 HOMO: -6.97428 LUMO: -1.22179 factor:1 | 1 (-0.47819) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.27778 HOMO: -6.93346 LUMO: -1.09934 factor:1 | 1 (-0.82105) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.67617 HOMO: -7.17292 LUMO: -1.11839 factor:1 | 1 (-2.21944) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27347 HOMO: -7.00965 LUMO: -1.23268 factor:1 | 1 (-1.81674) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47742 HOMO: -6.73210 LUMO: -1.12383 factor:1 | 1 (-2.02069) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.93477 HOMO: -7.61375 LUMO: -0.11973 factor:1 | 1 (-1.47804) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24109 HOMO: -7.42327 LUMO: 0.41906 factor:1 | 1 (-1.78436) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28558 HOMO: -6.94162 LUMO: -1.01771 factor:1 | 1 (-1.82885) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.20602 HOMO: -6.82189 LUMO: -0.92791 factor:1 | 1 (-1.74928) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92446 HOMO: -6.92258 LUMO: -1.73881 factor:1 | 1 (-1.46773) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02356 HOMO: -6.50896 LUMO: -1.60819 factor:1 | 1 (-1.56683) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74288 HOMO: -6.38379 LUMO: -2.18780 factor:1 | 1 (-1.28615) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16985 HOMO: -6.48992 LUMO: -0.97417 factor:1 | 1 (-1.71312) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44227 HOMO: -6.01644 LUMO: -0.04354 factor:1 | 1 (-0.98554) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36690 HOMO: -6.70761 LUMO: -0.14422 factor:1 | 1 (-0.91017) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.86376 HOMO: -6.70216 LUMO: 0.14422 factor:1 | 1 (-0.40703) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15043 HOMO: -7.07224 LUMO: -0.10885 factor:1 | 1 (-0.69370) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.47558 HOMO: -7.52667 LUMO: -0.74287 factor:1 | 1 (-1.01885) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55945 HOMO: -6.48447 LUMO: -0.96056 factor:1 | 1 (-1.10271) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74087 HOMO: -6.22597 LUMO: -0.41361 factor:1 | 1 (-1.28413) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91254 HOMO: -6.12256 LUMO: -1.05852 factor:1 | 1 (-1.45581) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39217 HOMO: -6.97428 LUMO: -0.60681 factor:1 | 1 (-1.93544) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45666 HOMO: -6.78380 LUMO: -0.88981 factor:1 | 1 (-1.99993) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02263 HOMO: -6.85999 LUMO: 0.07891 factor:1 | 1 (-2.56590) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02990 HOMO: -7.08312 LUMO: -0.60137 factor:1 | 1 (-2.57316) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24746 HOMO: -6.57699 LUMO: -0.68028 factor:1 | 1 (-1.79073) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79479 HOMO: -6.09807 LUMO: -0.31837 factor:1 | 1 (-2.33806) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.49862 HOMO: -6.10624 LUMO: 0.14966 factor:1 | 1 (-2.04189) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.13491 HOMO: -6.77019 LUMO: -0.95784 factor:1 | 1 (-1.67818) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.29655 HOMO: -5.93208 LUMO: -0.44627 factor:1 | 1 (-1.83982) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99883 HOMO: -6.12256 LUMO: -0.27756 factor:1 | 1 (-1.54210) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28585 HOMO: -5.98106 LUMO: -0.37824 factor:1 | 1 (-1.82912) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.21506 HOMO: -7.06408 LUMO: -1.12927 factor:1 | 1 (-0.75833) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29101 HOMO: -6.70761 LUMO: -0.98505 factor:1 | 1 (-0.83427) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.22760 HOMO: -7.00965 LUMO: -0.42722 factor:1 | 1 (-0.77087) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15109 HOMO: -5.96201 LUMO: -0.59049 factor:1 | 1 (-0.69435) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16891 HOMO: -6.34570 LUMO: -1.68438 factor:1 | 1 (-0.71218) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.05182 HOMO: -6.97156 LUMO: -1.85854 factor:1 | 1 (-0.59509) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45805 HOMO: -5.91848 LUMO: -2.51433 factor:1 | 1 (-2.00132) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.01395 HOMO: -6.39195 LUMO: -1.66262 factor:1 | 1 (-2.55722) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.74042 HOMO: -6.50352 LUMO: 0.19592 factor:1 | 1 (-2.28369) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12012 HOMO: -6.45998 LUMO: 0.34831 factor:1 | 1 (-0.66339) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.69291 HOMO: -7.05319 LUMO: 0.23402 factor:1 | 1 (-2.23618) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39290 HOMO: -6.61237 LUMO: 0.18232 factor:1 | 1 (-1.93617) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48886 HOMO: -6.57427 LUMO: 0.40545 factor:1 | 1 (-1.03213) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.54763 HOMO: -7.26544 LUMO: 0.41089 factor:1 | 1 (-2.09090) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78378 HOMO: -6.26406 LUMO: -0.85444 factor:1 | 1 (-1.32704) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11225 HOMO: -6.25318 LUMO: -0.79457 factor:1 | 1 (-1.65551) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15930 HOMO: -6.68040 LUMO: 0.41089 factor:1 | 1 (-0.70257) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19441 HOMO: -6.37835 LUMO: 0.37280 factor:1 | 1 (-0.73767) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.23299 HOMO: -6.56067 LUMO: 0.62858 factor:1 | 1 (-0.77626) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.31601 HOMO: -6.74026 LUMO: -0.04082 factor:1 | 1 (-0.85928) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15661 HOMO: -6.53617 LUMO: 0.35103 factor:1 | 1 (-0.69988) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26423 HOMO: -6.51985 LUMO: 0.25851 factor:1 | 1 (-0.80750) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38249 HOMO: -6.58788 LUMO: -1.98371 factor:1 | 1 (-0.92576) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.99631 HOMO: -6.51441 LUMO: 0.29116 factor:1 | 1 (-0.53957) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.27751 HOMO: -6.81101 LUMO: 0.35647 factor:1 | 1 (-0.82078) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.97764 HOMO: -6.42733 LUMO: 0.10340 factor:1 | 1 (-0.52091) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.18763 HOMO: -6.70761 LUMO: 0.28028 factor:1 | 1 (-0.73090) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.03413 HOMO: -6.67495 LUMO: 0.01633 factor:1 | 1 (-0.57740) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.14597 HOMO: -6.75387 LUMO: 0.15510 factor:1 | 1 (-0.68924) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32722 HOMO: -6.56067 LUMO: 0.35919 factor:1 | 1 (-0.87049) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32118 HOMO: -7.16748 LUMO: 0.21497 factor:1 | 1 (-0.86445) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.29762 HOMO: -6.71849 LUMO: 0.26667 factor:1 | 1 (-0.84089) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.35191 HOMO: -6.69128 LUMO: 0.55783 factor:1 | 1 (-0.89517) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10613 HOMO: -6.71305 LUMO: 0.45987 factor:1 | 1 (-0.64940) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.99032 HOMO: -5.90487 LUMO: -0.70750 factor:1 | 1 (-0.53359) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.11903 HOMO: -6.84638 LUMO: -0.72110 factor:1 | 1 (-0.66230) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20641 HOMO: -6.66135 LUMO: -1.13471 factor:1 | 1 (-0.74967) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.23065 HOMO: -6.74026 LUMO: -0.64763 factor:1 | 1 (-0.77392) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84772 HOMO: -6.69672 LUMO: -1.05036 factor:1 | 1 (-1.39099) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.84225 HOMO: -6.78924 LUMO: -1.03675 factor:1 | 1 (-1.38552) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95804 HOMO: -6.81373 LUMO: -0.85988 factor:1 | 1 (-1.50131) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89110 HOMO: -7.26544 LUMO: 0.91158 factor:1 | 1 (-1.43437) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32540 HOMO: -6.64230 LUMO: -1.92929 factor:1 | 1 (-0.86867) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.33860 HOMO: -7.20830 LUMO: 0.11429 factor:1 | 1 (-0.88187) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.95103 HOMO: -7.17020 LUMO: 0.04898 factor:1 | 1 (-0.49429) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.20390 HOMO: -7.16476 LUMO: 0.04898 factor:1 | 1 (-0.74717) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.66149 HOMO: -6.59332 LUMO: -0.49253 factor:1 | 1 (-1.20476) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.80655 HOMO: -7.46953 LUMO: 0.84083 factor:1 | 1 (-1.34982) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.70359 HOMO: -7.39878 LUMO: 0.88709 factor:1 | 1 (-1.24685) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.71211 HOMO: -6.84094 LUMO: -0.61498 factor:1 | 1 (-0.25538) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.97443 HOMO: -6.03549 LUMO: -0.27211 factor:1 | 1 (-0.51770) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.19811 HOMO: -7.31170 LUMO: -0.64763 factor:1 | 1 (-0.74137) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.99636 HOMO: -6.88992 LUMO: -0.84627 factor:1 | 1 (-0.53963) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.41661 HOMO: -7.12666 LUMO: -0.09252 factor:1 | 1 (-0.95988) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55313 HOMO: -6.70489 LUMO: -0.63675 factor:1 | 1 (-1.09640) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53368 HOMO: -6.98788 LUMO: 0.86804 factor:1 | 1 (-1.07695) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.49403 HOMO: -6.80285 LUMO: -0.60954 factor:1 | 1 (-1.03730) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02609 HOMO: -7.02054 LUMO: -0.74287 factor:1 | 1 (-1.56936) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99331 HOMO: -7.03686 LUMO: -0.81090 factor:1 | 1 (-1.53657) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91513 HOMO: -6.70489 LUMO: -1.00954 factor:1 | 1 (-1.45839) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87646 HOMO: -7.69810 LUMO: 0.00544 factor:1 | 1 (-1.41973) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96890 HOMO: -6.83550 LUMO: -0.11157 factor:1 | 1 (-1.51216) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95948 HOMO: -6.76203 LUMO: -2.13609 factor:1 | 1 (-1.50275) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82661 HOMO: -6.72121 LUMO: -2.62862 factor:1 | 1 (-1.36988) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37893 HOMO: -6.48719 LUMO: -2.73474 factor:1 | 1 (-0.92219) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.11280 HOMO: -6.83006 LUMO: -0.00544 factor:1 | 1 (-0.65607) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.23784 HOMO: -6.84094 LUMO: -1.11022 factor:1 | 1 (-0.78110) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36646 HOMO: -6.66951 LUMO: -1.23812 factor:1 | 1 (-0.90973) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33119 HOMO: -6.78380 LUMO: -1.27894 factor:1 | 1 (-1.87446) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36417 HOMO: -6.50352 LUMO: -0.56055 factor:1 | 1 (-1.90744) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31282 HOMO: -7.77974 LUMO: -0.26395 factor:1 | 1 (-1.85609) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57008 HOMO: -7.01510 LUMO: -1.64085 factor:1 | 1 (-2.11335) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47103 HOMO: -6.59876 LUMO: -0.91158 factor:1 | 1 (-2.01430) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55476 HOMO: -4.67219 LUMO: -0.67756 factor:1 | 1 (-2.09803) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.63914 HOMO: -6.70489 LUMO: -0.65579 factor:1 | 1 (-2.18241) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.37704 HOMO: -6.62325 LUMO: -0.60409 factor:1 | 1 (-1.92031) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08550 HOMO: -6.20147 LUMO: 0.15238 factor:1 | 1 (-1.62876) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04199 HOMO: -6.43549 LUMO: -0.07075 factor:1 | 1 (-1.58525) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15048 HOMO: -7.02054 LUMO: 0.13061 factor:1 | 1 (-1.69375) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.82046 HOMO: -7.04503 LUMO: 0.30749 factor:1 | 1 (-1.36373) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96307 HOMO: -6.74842 LUMO: -0.99594 factor:1 | 1 (-1.50634) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.06656 HOMO: -6.35658 LUMO: 0.41633 factor:1 | 1 (-1.60983) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98599 HOMO: -6.79740 LUMO: 0.56872 factor:1 | 1 (-1.52925) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.81549 HOMO: -6.51713 LUMO: -0.05987 factor:1 | 1 (-3.35876) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10105 HOMO: -6.68040 LUMO: 0.34558 factor:1 | 1 (-2.64432) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.81864 HOMO: -6.39740 LUMO: 0.50069 factor:1 | 1 (-3.36191) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14171 HOMO: -6.91713 LUMO: -0.97145 factor:1 | 1 (-2.68497) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10149 HOMO: -7.10761 LUMO: -0.27483 factor:1 | 1 (-2.64476) | 1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.67225 HOMO: -6.98788 LUMO: 0.40273 factor:1 | 1 (-3.21552) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23156 HOMO: -6.87087 LUMO: 0.28572 factor:1 | 1 (-2.77483) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33581 HOMO: -7.36612 LUMO: -0.12245 factor:1 | 1 (-2.87907) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.61559 HOMO: -6.72938 LUMO: 0.33742 factor:1 | 1 (-3.15886) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.99361 HOMO: -7.32531 LUMO: 0.07619 factor:1 | 1 (-3.53688) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.12756 HOMO: -6.87087 LUMO: -0.08436 factor:1 | 1 (-2.67082) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05330 HOMO: -6.67495 LUMO: 0.85988 factor:1 | 1 (-2.59656) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.46797 HOMO: -6.96339 LUMO: 0.65307 factor:1 | 1 (-3.01124) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11371 HOMO: -6.58516 LUMO: -0.78641 factor:1 | 1 (-2.65697) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.67472 HOMO: -6.56883 LUMO: 0.44355 factor:1 | 1 (-3.21799) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15637 HOMO: -6.68312 LUMO: 0.43538 factor:1 | 1 (-2.69964) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18345 HOMO: -6.81917 LUMO: 0.20681 factor:1 | 1 (-2.72672) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15624 HOMO: -6.91169 LUMO: 0.08163 factor:1 | 1 (-2.69951) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96666 HOMO: -4.88444 LUMO: -0.49253 factor:1 | 1 (-2.50992) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79786 HOMO: -6.42189 LUMO: 0.64763 factor:1 | 1 (-2.34113) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06176 HOMO: -6.24501 LUMO: 0.55783 factor:1 | 1 (-2.60503) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.28400 HOMO: -6.41372 LUMO: 0.29388 factor:1 | 1 (-2.82726) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24877 HOMO: -5.67902 LUMO: 1.77690 factor:1 | 1 (-1.79203) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42425 HOMO: -6.55794 LUMO: 0.05170 factor:1 | 1 (-1.96752) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.85906 HOMO: -6.52801 LUMO: 0.25851 factor:1 | 1 (-2.40233) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93019 HOMO: -7.08857 LUMO: 0.11157 factor:1 | 1 (-2.47346) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93368 HOMO: -6.58243 LUMO: 0.75648 factor:1 | 1 (-2.47694) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.91686 HOMO: -7.22190 LUMO: 0.45171 factor:1 | 1 (-2.46013) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.55544 HOMO: -6.47087 LUMO: 0.00000 factor:1 | 1 (-2.09871) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.83925 HOMO: -6.78652 LUMO: 1.32247 factor:1 | 1 (-2.38252) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.86527 HOMO: -6.74026 LUMO: 1.45309 factor:1 | 1 (-2.40853) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.73601 HOMO: -6.69944 LUMO: 0.76464 factor:1 | 1 (-2.27928) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.34088 HOMO: -6.62325 LUMO: 0.64763 factor:1 | 1 (-1.88414) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33318 HOMO: -6.45182 LUMO: 0.49253 factor:1 | 1 (-1.87644) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16066 HOMO: -7.14843 LUMO: 0.62586 factor:1 | 1 (-1.70392) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15519 HOMO: -6.87087 LUMO: 1.53200 factor:1 | 1 (-1.69845) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31312 HOMO: -6.54978 LUMO: 0.45171 factor:1 | 1 (-1.85639) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.26166 HOMO: -6.63686 LUMO: 0.80001 factor:1 | 1 (-1.80493) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08972 HOMO: -7.00693 LUMO: 1.56193 factor:1 | 1 (-1.63298) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24419 HOMO: -6.02460 LUMO: 1.72792 factor:1 | 1 (-1.78746) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.38554 HOMO: -6.36746 LUMO: -1.20002 factor:1 | 1 (-0.92881) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.93339 HOMO: -7.26816 LUMO: -1.06397 factor:1 | 1 (-0.47666) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09634 HOMO: -7.34707 LUMO: -1.09662 factor:1 | 1 (-0.63960) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.11035 HOMO: -7.93212 LUMO: -0.13606 factor:1 | 1 (-0.65362) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.98825 HOMO: -6.80285 LUMO: 0.58504 factor:1 | 1 (-0.53152) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13435 HOMO: -7.12938 LUMO: 0.32926 factor:1 | 1 (-0.67762) | 1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30709 HOMO: -6.86815 LUMO: -1.30070 factor:1 | 1 (-0.85036) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.08537 HOMO: -6.99333 LUMO: -1.03947 factor:1 | 1 (-0.62864) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42297 HOMO: -7.56749 LUMO: -0.11157 factor:1 | 1 (-1.96624) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33984 HOMO: -7.57293 LUMO: -0.07891 factor:1 | 1 (-1.88311) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11976 HOMO: -7.30626 LUMO: 0.27211 factor:1 | 1 (-1.66302) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.85617 HOMO: -7.77974 LUMO: 0.27211 factor:1 | 1 (-0.39944) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.04330 HOMO: -7.11578 LUMO: 0.19864 factor:1 | 1 (-0.58657) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.07617 HOMO: -7.71171 LUMO: 0.57688 factor:1 | 1 (-0.61944) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75152 HOMO: -7.83688 LUMO: 0.37824 factor:1 | 1 (-2.29479) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53432 HOMO: -6.94979 LUMO: -1.66534 factor:1 | 1 (-2.07759) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90451 HOMO: -6.97156 LUMO: -1.13199 factor:1 | 1 (-1.44778) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72589 HOMO: -6.91441 LUMO: -1.08301 factor:1 | 1 (-2.26916) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01573 HOMO: -6.71849 LUMO: -0.74831 factor:1 | 1 (-1.55899) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05162 HOMO: -7.09401 LUMO: -1.77690 factor:1 | 1 (-1.59489) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17366 HOMO: -6.97156 LUMO: -1.45037 factor:1 | 1 (-1.71693) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03652 HOMO: -7.22462 LUMO: -1.11295 factor:1 | 1 (-1.57978) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98569 HOMO: -7.85321 LUMO: 0.16599 factor:1 | 1 (-1.52895) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02408 HOMO: -7.71987 LUMO: 0.55511 factor:1 | 1 (-1.56735) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98286 HOMO: -7.63551 LUMO: 0.14422 factor:1 | 1 (-1.52612) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94084 HOMO: -6.98788 LUMO: -0.80546 factor:1 | 1 (-1.48411) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99809 HOMO: -6.98788 LUMO: -1.16737 factor:1 | 1 (-1.54136) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.48807 HOMO: -6.56611 LUMO: -1.60819 factor:1 | 1 (-1.03134) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99883 HOMO: -6.95251 LUMO: 0.66396 factor:1 | 1 (-1.54210) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.70652 HOMO: -7.35252 LUMO: 0.49797 factor:1 | 1 (-1.24979) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96571 HOMO: -6.90897 LUMO: -0.81090 factor:1 | 1 (-1.50898) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.16569 HOMO: -7.04503 LUMO: -1.08301 factor:1 | 1 (-1.70896) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57245 HOMO: -6.92530 LUMO: -1.29526 factor:1 | 1 (-1.11572) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00691 HOMO: -6.93074 LUMO: -1.25444 factor:1 | 1 (-1.55018) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05717 HOMO: -6.73482 LUMO: -0.62042 factor:1 | 1 (-1.60044) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74489 HOMO: -7.67633 LUMO: 0.59593 factor:1 | 1 (-1.28816) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02057 HOMO: -7.39061 LUMO: -0.19320 factor:1 | 1 (-1.56384) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74764 HOMO: -7.55388 LUMO: -0.20136 factor:1 | 1 (-1.29091) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.79363 HOMO: -7.14027 LUMO: -0.99866 factor:1 | 1 (-1.33690) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97203 HOMO: -6.75931 LUMO: -0.73199 factor:1 | 1 (-1.51529) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.36546 HOMO: -5.45044 LUMO: -0.18776 factor:1 | 1 (-0.90872) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02612 HOMO: -6.70761 LUMO: -0.84083 factor:1 | 1 (-1.56939) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.56636 HOMO: -6.05453 LUMO: -1.06669 factor:1 | 1 (-1.10963) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94832 HOMO: -6.86815 LUMO: -0.98233 factor:1 | 1 (-1.49159) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.57482 HOMO: -6.73210 LUMO: -0.95240 factor:1 | 1 (-1.11809) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.77689 HOMO: -5.89671 LUMO: -1.05036 factor:1 | 1 (-1.32016) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88808 HOMO: -7.61102 LUMO: 0.33470 factor:1 | 1 (-1.43135) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91505 HOMO: -7.51034 LUMO: 0.23674 factor:1 | 1 (-1.45831) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83306 HOMO: -7.41510 LUMO: 0.62858 factor:1 | 1 (-1.37632) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94492 HOMO: -6.76203 LUMO: -1.72792 factor:1 | 1 (-1.48819) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.36115 HOMO: -6.60420 LUMO: -0.45715 factor:1 | 1 (-1.90442) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31671 HOMO: -6.59060 LUMO: -0.58232 factor:1 | 1 (-1.85998) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30262 HOMO: -7.43687 LUMO: -0.76736 factor:1 | 1 (-1.84588) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40945 HOMO: -6.08719 LUMO: -0.48708 factor:1 | 1 (-1.95272) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17018 HOMO: -5.88854 LUMO: -0.05714 factor:1 | 1 (-1.71345) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.85122 HOMO: -7.34435 LUMO: -0.71838 factor:1 | 1 (-3.39448) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.16431 HOMO: -7.46408 LUMO: -0.63130 factor:1 | 1 (-3.70758) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.62114 HOMO: -7.00965 LUMO: -1.24900 factor:1 | 1 (-3.16441) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.94599 HOMO: -6.91169 LUMO: -0.88981 factor:1 | 1 (-3.48926) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.17431 HOMO: -6.78652 LUMO: -0.82178 factor:1 | 1 (-2.71757) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.81530 HOMO: -7.80423 LUMO: 0.87076 factor:1 | 1 (-3.35857) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52131 HOMO: -6.97700 LUMO: -1.00954 factor:1 | 1 (-3.06457) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76513 HOMO: -6.92530 LUMO: -0.88165 factor:1 | 1 (-2.30840) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.22299 HOMO: -7.14571 LUMO: -1.04492 factor:1 | 1 (-2.76626) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.85802 HOMO: -7.49674 LUMO: 0.34558 factor:1 | 1 (-3.40129) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68275 HOMO: -6.44094 LUMO: -1.20819 factor:1 | 1 (-3.22602) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94641 HOMO: -6.47359 LUMO: -1.14016 factor:1 | 1 (-2.48968) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.53161 HOMO: -6.61237 LUMO: -0.87076 factor:1 | 1 (-1.07488) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94811 HOMO: -6.73754 LUMO: -1.09662 factor:1 | 1 (-1.49137) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.75099 HOMO: -6.97700 LUMO: 0.13061 factor:1 | 1 (-1.29426) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88724 HOMO: -6.82734 LUMO: 0.59865 factor:1 | 1 (-1.43050) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91850 HOMO: -6.86543 LUMO: -0.91430 factor:1 | 1 (-1.46177) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.78230 HOMO: -6.74298 LUMO: 0.28028 factor:1 | 1 (-2.32557) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47867 HOMO: -6.75387 LUMO: 0.19592 factor:1 | 1 (-2.02194) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.47038 HOMO: -7.05591 LUMO: 0.10612 factor:1 | 1 (-2.01364) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90641 HOMO: -6.86543 LUMO: 0.49253 factor:1 | 1 (-2.44968) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.66709 HOMO: -6.11440 LUMO: -1.12655 factor:1 | 1 (-2.21035) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.61171 HOMO: -6.77291 LUMO: -1.02859 factor:1 | 1 (-2.15498) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79452 HOMO: -6.54978 LUMO: 0.29116 factor:1 | 1 (-2.33778) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.61153 HOMO: -7.18108 LUMO: 0.00000 factor:1 | 1 (-1.15480) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.67482 HOMO: -6.86271 LUMO: -1.15376 factor:1 | 1 (-1.21809) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.85953 HOMO: -6.78108 LUMO: -1.22723 factor:1 | 1 (-1.40280) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01194 HOMO: -6.40828 LUMO: 0.02449 factor:1 | 1 (-1.55521) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.91330 HOMO: -6.43821 LUMO: 0.09796 factor:1 | 1 (-1.45657) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.65793 HOMO: -6.99877 LUMO: 0.40545 factor:1 | 1 (-3.20120) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.59562 HOMO: -6.68856 LUMO: 0.19320 factor:1 | 1 (-3.13889) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03224 HOMO: -7.11034 LUMO: 0.31293 factor:1 | 1 (-2.57550) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.41910 HOMO: -6.92530 LUMO: -0.85444 factor:1 | 1 (-2.96237) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.70148 HOMO: -6.60148 LUMO: -0.59865 factor:1 | 1 (-2.24475) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79781 HOMO: -6.72938 LUMO: 0.30749 factor:1 | 1 (-2.34108) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94813 HOMO: -7.31170 LUMO: 0.06803 factor:1 | 1 (-2.49139) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.81092 HOMO: -7.09129 LUMO: -0.04626 factor:1 | 1 (-3.35418) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06168 HOMO: -6.38379 LUMO: -0.76736 factor:1 | 1 (-2.60495) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14097 HOMO: -6.13617 LUMO: -0.63947 factor:1 | 1 (-2.68424) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10179 HOMO: -6.92258 LUMO: 0.37007 factor:1 | 1 (-2.64506) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17042 HOMO: -6.35930 LUMO: 0.41361 factor:1 | 1 (-1.71369) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13732 HOMO: -6.60420 LUMO: 0.26667 factor:1 | 1 (-0.68058) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.50277 HOMO: -6.04909 LUMO: 1.82588 factor:1 | 1 (-1.04603) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52027 HOMO: -6.69672 LUMO: 1.72520 factor:1 | 1 (-3.06354) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15556 HOMO: -6.50080 LUMO: 0.29116 factor:1 | 1 (-2.69883) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.35782 HOMO: -6.60692 LUMO: -0.43266 factor:1 | 1 (-2.90109) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.02450 HOMO: -6.93890 LUMO: 0.39729 factor:1 | 1 (-3.56777) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.15536 HOMO: -6.52801 LUMO: -0.47076 factor:1 | 1 (-3.69863) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.31681 HOMO: -6.41100 LUMO: 0.30477 factor:1 | 1 (-2.86008) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37877 HOMO: -6.37291 LUMO: -0.80001 factor:1 | 1 (-2.92204) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.07528 HOMO: -6.51985 LUMO: 1.44765 factor:1 | 1 (-3.61854) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.98181 HOMO: -6.64774 LUMO: 0.04626 factor:1 | 1 (-2.52508) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45835 HOMO: -6.65863 LUMO: 0.29933 factor:1 | 1 (-2.00162) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15839 HOMO: -7.09673 LUMO: 0.28300 factor:1 | 1 (-2.70166) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27725 HOMO: -6.57155 LUMO: -1.11567 factor:1 | 1 (-2.82051) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08313 HOMO: -6.38379 LUMO: -0.60681 factor:1 | 1 (-1.62640) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14830 HOMO: -6.60148 LUMO: 0.18232 factor:1 | 1 (-1.69157) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.52787 HOMO: -6.96067 LUMO: -0.52246 factor:1 | 1 (-2.07114) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.39146 HOMO: -6.57427 LUMO: -0.84627 factor:1 | 1 (-1.93473) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.34571 HOMO: -6.59332 LUMO: -0.98233 factor:1 | 1 (-2.88898) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.16693 HOMO: -6.20692 LUMO: -0.27483 factor:1 | 1 (-2.71020) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.21494 HOMO: -6.81373 LUMO: 0.74559 factor:1 | 1 (-1.75821) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09570 HOMO: -6.60420 LUMO: 0.54695 factor:1 | 1 (-1.63897) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.59313 HOMO: -6.58788 LUMO: -0.31021 factor:1 | 1 (-2.13639) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99498 HOMO: -6.72938 LUMO: 0.64763 factor:1 | 1 (-2.53825) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.00913 HOMO: -6.86815 LUMO: 0.32109 factor:1 | 1 (-2.55240) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.96471 HOMO: -6.63141 LUMO: 0.18776 factor:1 | 1 (-1.50797) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94299 HOMO: -7.18653 LUMO: 0.09524 factor:1 | 1 (-1.48626) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22400 HOMO: -6.83550 LUMO: 0.03537 factor:1 | 1 (-1.76727) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.21015 HOMO: -7.47769 LUMO: 0.40817 factor:1 | 1 (-1.75342) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.64408 HOMO: -6.57971 LUMO: -0.63675 factor:1 | 1 (-3.18735) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.37887 HOMO: -6.74842 LUMO: -0.16327 factor:1 | 1 (-3.92214) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.28065 HOMO: -7.07224 LUMO: 0.61770 factor:1 | 1 (-2.82392) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07556 HOMO: -6.83006 LUMO: 0.54695 factor:1 | 1 (-2.61882) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.95107 HOMO: -6.60148 LUMO: 1.23540 factor:1 | 1 (-1.49434) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.58526 HOMO: -6.99061 LUMO: 0.41089 factor:1 | 1 (-2.12853) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.30224 HOMO: -6.63686 LUMO: 0.85172 factor:1 | 1 (-1.84550) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.97409 HOMO: -6.50624 LUMO: 0.12517 factor:1 | 1 (-2.51735) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.82273 HOMO: -6.35658 LUMO: 0.36463 factor:1 | 1 (-3.36599) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.02009 HOMO: -6.34570 LUMO: 0.65035 factor:1 | 1 (-3.56336) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.11304 HOMO: -6.63141 LUMO: 1.25717 factor:1 | 1 (-3.65631) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.06726 HOMO: -6.91441 LUMO: 1.32792 factor:1 | 1 (-2.61052) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33668 HOMO: -7.15387 LUMO: 0.64219 factor:1 | 1 (-2.87994) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02990 HOMO: -7.17836 LUMO: 0.60409 factor:1 | 1 (-2.57316) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25020 HOMO: -6.92258 LUMO: 0.49525 factor:1 | 1 (-2.79347) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88233 HOMO: -6.31032 LUMO: 0.48708 factor:1 | 1 (-2.42560) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.80674 HOMO: -6.49808 LUMO: 0.31021 factor:1 | 1 (-2.35000) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.04570 HOMO: -6.48447 LUMO: 0.37552 factor:1 | 1 (-0.58896) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.18121 HOMO: -6.66135 LUMO: -1.08301 factor:1 | 1 (-0.72448) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.05454 HOMO: -6.33481 LUMO: -0.51974 factor:1 | 1 (-0.59781) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.30140 HOMO: -6.76475 LUMO: -0.15238 factor:1 | 1 (-0.84467) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03896 HOMO: -6.93346 LUMO: -0.10885 factor:1 | 1 (-2.58222) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23322 HOMO: -7.19741 LUMO: 0.73199 factor:1 | 1 (-2.77649) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.92611 HOMO: -6.82734 LUMO: 0.88437 factor:1 | 1 (-2.46938) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.88059 HOMO: -7.01237 LUMO: 0.02721 factor:1 | 1 (-2.42385) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.01141 HOMO: -6.39195 LUMO: 1.46941 factor:1 | 1 (-0.55468) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.15441 HOMO: -6.53890 LUMO: 1.32792 factor:1 | 1 (-0.69767) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27186 HOMO: -6.82734 LUMO: 1.98099 factor:1 | 1 (-2.81513) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.21145 HOMO: -6.74570 LUMO: 1.68983 factor:1 | 1 (-2.75472) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.11469 HOMO: -6.41100 LUMO: 1.39050 factor:1 | 1 (-2.65795) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.83855 HOMO: -5.92664 LUMO: 1.65989 factor:1 | 1 (-1.38182) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.70889 HOMO: -6.07630 LUMO: 1.54833 factor:1 | 1 (-1.25216) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89654 HOMO: -6.45998 LUMO: 0.68573 factor:1 | 1 (-1.43981) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.57785 HOMO: -6.52801 LUMO: 0.41361 factor:1 | 1 (-3.12112) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90206 HOMO: -6.77564 LUMO: 0.42178 factor:1 | 1 (-2.44532) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.75936 HOMO: -6.56339 LUMO: 1.65717 factor:1 | 1 (-2.30263) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.89466 HOMO: -5.85861 LUMO: 1.90752 factor:1 | 1 (-2.43792) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.10557 HOMO: -6.77019 LUMO: -2.48440 factor:1 | -1 (0.35116) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.36568 HOMO: -6.53890 LUMO: -1.82588 factor:1 | -1 (0.09105) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.64373 HOMO: -6.50352 LUMO: -1.66806 factor:1 | 1 (-0.18700) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.79271 HOMO: -6.90625 LUMO: 0.43538 factor:1 | 1 (-0.33598) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.46887 HOMO: -6.85455 LUMO: 0.53062 factor:1 | 1 (-3.01214) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.25186 HOMO: -6.49536 LUMO: 0.31021 factor:1 | 1 (-2.79513) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.49655 HOMO: -4.97696 LUMO: -0.09252 factor:1 | 1 (-2.03982) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.72434 HOMO: -5.31166 LUMO: 0.34286 factor:1 | 1 (-2.26761) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17061 HOMO: -6.42461 LUMO: 0.74287 factor:1 | 1 (-1.71388) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99692 HOMO: -6.59604 LUMO: 0.62858 factor:1 | 1 (-1.54019) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05535 HOMO: -6.45998 LUMO: -0.61770 factor:1 | 1 (-1.59861) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.18830 HOMO: -6.75659 LUMO: -0.34014 factor:1 | 1 (-1.73157) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.99957 HOMO: -6.63958 LUMO: 0.36191 factor:1 | 1 (-0.54284) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.26975 HOMO: -5.92936 LUMO: -0.67484 factor:1 | 1 (-0.81302) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.23088 HOMO: -5.67630 LUMO: 1.80956 factor:1 | 1 (-2.77415) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.46009 HOMO: -6.50352 LUMO: -0.78369 factor:1 | 1 (-2.00336) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.33630 HOMO: -6.35930 LUMO: -0.75648 factor:1 | 1 (-2.87956) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18535 HOMO: -6.74298 LUMO: 0.48980 factor:1 | 1 (-2.72862) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.00753 HOMO: -6.85183 LUMO: 0.15510 factor:1 | 1 (-2.55080) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.23905 HOMO: -6.90897 LUMO: 0.26123 factor:1 | 1 (-1.78232) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.37549 HOMO: -6.85999 LUMO: 0.47892 factor:1 | 1 (-1.91876) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.57008 HOMO: -6.69944 LUMO: 0.57416 factor:1 | 1 (-2.11335) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42923 HOMO: -6.74026 LUMO: 0.69933 factor:1 | 1 (-1.97250) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.17105 HOMO: -6.52801 LUMO: 0.75376 factor:1 | 1 (-1.71432) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.83919 HOMO: -7.05863 LUMO: 0.44627 factor:1 | 1 (-0.38246) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.02872 HOMO: -6.96339 LUMO: 0.48164 factor:1 | 1 (-0.57198) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31766 HOMO: -6.95795 LUMO: 0.44355 factor:1 | 1 (-1.86093) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.14944 HOMO: -6.36746 LUMO: 0.58777 factor:1 | 1 (-1.69271) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03649 HOMO: -6.69400 LUMO: 0.40545 factor:1 | 1 (-1.57976) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.99426 HOMO: -6.30760 LUMO: -0.66668 factor:1 | 1 (-1.53752) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.20757 HOMO: -6.53617 LUMO: -0.64491 factor:1 | 1 (-1.75083) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45184 HOMO: -6.80829 LUMO: 0.17415 factor:1 | 1 (-1.99511) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86383 HOMO: -6.80285 LUMO: 0.73471 factor:1 | 1 (-1.40710) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.62641 HOMO: -6.43821 LUMO: 0.21769 factor:1 | 1 (-2.16967) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.04136 HOMO: -6.98788 LUMO: 0.10885 factor:1 | 1 (-1.58463) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89396 HOMO: -7.15115 LUMO: 0.40817 factor:1 | 1 (-1.43722) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.87956 HOMO: -6.00011 LUMO: -0.98505 factor:1 | 1 (-1.42283) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.74685 HOMO: -6.16882 LUMO: -0.77825 factor:1 | 1 (-1.29012) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11048 HOMO: -6.30760 LUMO: 0.34831 factor:1 | 1 (-1.65374) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92008 HOMO: -6.64502 LUMO: 0.63403 factor:1 | 1 (-1.46335) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.29246 HOMO: -6.93618 LUMO: 0.96600 factor:1 | -1 (0.16428) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.59088 HOMO: -6.45182 LUMO: 0.16327 factor:1 | 1 (-0.13415) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.75350 HOMO: -6.99605 LUMO: 0.20953 factor:1 | 1 (-0.29677) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.05816 HOMO: -6.72665 LUMO: 0.32654 factor:1 | 1 (-0.60143) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.08387 HOMO: -6.38379 LUMO: 0.45443 factor:1 | 1 (-0.62714) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.34791 HOMO: -6.65318 LUMO: 0.04354 factor:1 | 1 (-0.89117) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09821 HOMO: -6.94707 LUMO: -1.68438 factor:1 | 1 (-0.64148) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.37014 HOMO: -6.71849 LUMO: 0.15783 factor:1 | 1 (-0.91340) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.44614 HOMO: -6.97156 LUMO: 0.43266 factor:1 | 1 (-0.98941) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.67820 HOMO: -6.91441 LUMO: -0.54695 factor:1 | 1 (-1.22146) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.69325 HOMO: -6.74842 LUMO: -0.76192 factor:1 | 1 (-1.23651) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92819 HOMO: -6.70489 LUMO: 0.19048 factor:1 | 1 (-1.47146) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.80697 HOMO: -7.25728 LUMO: 0.33470 factor:1 | 1 (-0.35024) | 1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.70365 HOMO: -6.96339 LUMO: 0.55511 factor:1 | 1 (-0.24692) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.75872 HOMO: -6.77564 LUMO: 0.72382 factor:1 | 1 (-0.30199) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91021 HOMO: -6.75387 LUMO: 0.39729 factor:1 | 1 (-0.45348) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.02940 HOMO: -7.00149 LUMO: 0.06531 factor:1 | 1 (-0.57266) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.89122 HOMO: -7.09945 LUMO: 0.33470 factor:1 | 1 (-0.43448) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.12426 HOMO: -7.20830 LUMO: 0.59593 factor:1 | 1 (-0.66752) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97352 HOMO: -6.40556 LUMO: 0.56600 factor:1 | 1 (-1.51679) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86049 HOMO: -6.77291 LUMO: 0.73471 factor:1 | 1 (-1.40375) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10727 HOMO: -6.65046 LUMO: 0.09796 factor:1 | 1 (-1.65053) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.37491 HOMO: -6.95795 LUMO: 0.22313 factor:1 | 1 (-2.91818) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27629 HOMO: -6.85727 LUMO: 0.04626 factor:1 | 1 (-2.81956) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.42344 HOMO: -7.27360 LUMO: 0.42178 factor:1 | 1 (-1.96670) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.08786 HOMO: -6.78924 LUMO: -0.13334 factor:1 | 1 (-2.63112) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24036 HOMO: -6.63141 LUMO: 0.38368 factor:1 | 1 (-1.78362) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50534 HOMO: -6.92258 LUMO: 0.39184 factor:1 | 1 (-2.04861) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.14429 HOMO: -6.19331 LUMO: -0.46804 factor:1 | -1 (0.31244) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.01264 HOMO: -7.26544 LUMO: -0.05442 factor:1 | -1 (0.44409) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.21159 HOMO: -7.09401 LUMO: 0.30749 factor:1 | -1 (0.24515) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13277 HOMO: -6.14705 LUMO: -0.88709 factor:1 | 1 (-0.67604) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.95255 HOMO: -6.53617 LUMO: -0.28572 factor:1 | 1 (-0.49582) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.16126 HOMO: -6.37291 LUMO: -0.67212 factor:1 | 1 (-0.70453) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.80066 HOMO: -6.65591 LUMO: 0.03810 factor:1 | 1 (-0.34392) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.61755 HOMO: -7.11034 LUMO: 0.75103 factor:1 | 1 (-0.16082) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.84907 HOMO: -6.85183 LUMO: -0.05987 factor:1 | 1 (-0.39233) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.39076 HOMO: -6.70761 LUMO: -0.05442 factor:1 | 1 (-0.93403) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.32137 HOMO: -6.23413 LUMO: 0.06259 factor:1 | 1 (-0.86464) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.55460 HOMO: -6.55794 LUMO: 0.74015 factor:1 | 1 (-1.09787) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.36911 HOMO: -7.27905 LUMO: 0.26939 factor:1 | 1 (-2.91238) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.38422 HOMO: -6.34842 LUMO: -0.86804 factor:1 | 1 (-2.92748) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45623 HOMO: -6.27222 LUMO: 1.46125 factor:1 | 1 (-1.99949) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27794 HOMO: -6.65046 LUMO: 2.04902 factor:1 | 1 (-1.82120) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.09567 HOMO: -7.11850 LUMO: -1.14016 factor:1 | 1 (-2.63893) | 1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.45756 HOMO: -6.88720 LUMO: -1.20274 factor:1 | 1 (-2.00083) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53059 HOMO: -6.69400 LUMO: -0.31565 factor:1 | 1 (-2.07386) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38134 HOMO: -6.95523 LUMO: -1.55377 factor:1 | 1 (-1.92461) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.28365 HOMO: -6.41372 LUMO: -0.83539 factor:1 | 1 (-1.82692) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.25554 HOMO: -6.13889 LUMO: -0.90070 factor:1 | 1 (-1.79881) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.50651 HOMO: -6.44366 LUMO: -0.55511 factor:1 | 1 (-2.04978) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.90781 HOMO: -6.10079 LUMO: -0.71022 factor:1 | 1 (-1.45107) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.15015 HOMO: -6.90353 LUMO: -0.64763 factor:1 | 1 (-1.69342) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33560 HOMO: -6.65046 LUMO: -0.82450 factor:1 | 1 (-1.87886) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.22896 HOMO: -6.81645 LUMO: -0.85444 factor:1 | 1 (-1.77222) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.03801 HOMO: -6.20692 LUMO: 1.30887 factor:1 | 1 (-1.58128) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.05872 HOMO: -5.96201 LUMO: 1.33880 factor:1 | 1 (-1.60199) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.27976 HOMO: -6.52529 LUMO: 1.58914 factor:1 | 1 (-1.82303) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.86379 HOMO: -6.58516 LUMO: 1.97555 factor:1 | 1 (-0.40706) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.14265 HOMO: -6.84366 LUMO: 0.15783 factor:1 | 1 (-0.68592) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.38501 HOMO: -6.45726 LUMO: 0.42994 factor:1 | 1 (-1.92828) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.10787 HOMO: -6.75387 LUMO: 0.14422 factor:1 | 1 (-1.65113) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.81818 HOMO: -6.69944 LUMO: 1.79051 factor:1 | 1 (-0.36145) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.07549 HOMO: -6.59876 LUMO: 1.90208 factor:1 | 1 (-0.61876) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.40327 HOMO: -7.05863 LUMO: 1.20819 factor:1 | 1 (-1.94654) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.32507 HOMO: -6.54978 LUMO: 2.01636 factor:1 | 1 (-1.86833) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.81493 HOMO: -5.52119 LUMO: 1.95106 factor:1 | 1 (-1.35820) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.53266 HOMO: -6.53617 LUMO: 1.60275 factor:1 | 1 (-2.07593) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.08729 HOMO: -6.11440 LUMO: 1.89119 factor:1 | 1 (-1.63056) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.66033 HOMO: -7.31986 LUMO: 0.48708 factor:1 | 1 (-0.20360) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.91783 HOMO: -6.76475 LUMO: -0.75648 factor:1 | 1 (-0.46110) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.73048 HOMO: -6.76747 LUMO: -1.06941 factor:1 | 1 (-0.27375) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.97043 HOMO: -6.87087 LUMO: 0.72927 factor:1 | 1 (-0.51370) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.46992 HOMO: -7.00965 LUMO: 0.02177 factor:1 | 1 (-1.01319) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.75706 HOMO: -6.54706 LUMO: -0.03265 factor:1 | 1 (-1.30032) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.84675 HOMO: -6.62325 LUMO: -0.63675 factor:1 | 1 (-0.39002) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.10099 HOMO: -7.03414 LUMO: -1.24084 factor:1 | 1 (-0.64426) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.34127 HOMO: -7.04503 LUMO: -0.10068 factor:1 | 1 (-3.88453) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.98145 HOMO: -6.67223 LUMO: 0.03537 factor:1 | 1 (-3.52472) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.31891 HOMO: -6.82734 LUMO: 0.58777 factor:1 | 1 (-2.86218) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.14771 HOMO: -6.84366 LUMO: 0.46531 factor:1 | 1 (-3.69098) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.76460 HOMO: -7.03959 LUMO: -1.15104 factor:1 | 1 (-3.30787) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.81716 HOMO: -6.91169 LUMO: -0.41361 factor:1 | 1 (-2.36042) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68678 HOMO: -7.10217 LUMO: -0.44627 factor:1 | 1 (-3.23005) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.61774 HOMO: -6.88176 LUMO: -0.19592 factor:1 | 1 (-3.16101) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.02971 HOMO: -7.21374 LUMO: -0.46531 factor:1 | 1 (-2.57297) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.90327 HOMO: -6.54978 LUMO: 0.16871 factor:1 | 1 (-3.44654) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.77100 HOMO: -6.71305 LUMO: -0.13061 factor:1 | 1 (-3.31427) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.88629 HOMO: -6.74842 LUMO: -0.36191 factor:1 | 1 (-0.42956) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.13128 HOMO: -6.74570 LUMO: -0.09796 factor:1 | 1 (-0.67454) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98792 HOMO: -6.93890 LUMO: -0.27211 factor:1 | 1 (-1.53118) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.78190 HOMO: -6.88720 LUMO: -0.18776 factor:1 | 1 (-1.32517) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.75093 HOMO: -6.74842 LUMO: 0.02993 factor:1 | 1 (-1.29420) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.88136 HOMO: -6.70216 LUMO: 0.01361 factor:1 | 1 (-1.42462) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.01156 HOMO: -6.90625 LUMO: 0.00544 factor:1 | 1 (-1.55483) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94299 HOMO: -6.18243 LUMO: 0.25851 factor:1 | 1 (-1.48626) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.67063 HOMO: -6.32937 LUMO: -0.20953 factor:1 | 1 (-1.21390) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.89306 HOMO: -6.78108 LUMO: 0.00544 factor:1 | 1 (-1.43633) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.84828 HOMO: -5.97562 LUMO: 0.28572 factor:1 | 1 (-3.39155) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.68161 HOMO: -5.97290 LUMO: -0.18504 factor:1 | 1 (-3.22488) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.79746 HOMO: -6.12800 LUMO: 0.42178 factor:1 | 1 (-2.34072) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.15145 HOMO: -6.24229 LUMO: -0.00816 factor:1 | 1 (-2.69472) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.52256 HOMO: -6.61781 LUMO: 0.12789 factor:1 | 1 (-3.06583) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.76129 HOMO: -6.70489 LUMO: 0.14694 factor:1 | 1 (-2.30456) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.77384 HOMO: -6.86543 LUMO: -0.21225 factor:1 | 1 (-2.31710) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.81040 HOMO: -6.90081 LUMO: -0.20136 factor:1 | 1 (-3.35367) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.94413 HOMO: -7.12938 LUMO: -0.25851 factor:1 | 1 (-2.48739) | 1 | 1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.03934 HOMO: -6.93074 LUMO: -0.26667 factor:1 | 1 (-2.58261) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.51037 HOMO: -7.00421 LUMO: -0.31021 factor:1 | 1 (-3.05363) | -1 | -1 |
| G: -6256.09104 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.12788 HOMO: -7.10761 LUMO: -0.17415 factor:1 | 1 (-3.67114) | 1 | 1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.28857 HOMO: -8.21240 LUMO: 0.05987 factor:1 | 1 (-2.83183) | 1 | 1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.30386 HOMO: -7.14843 LUMO: -0.46531 factor:1 | 1 (-2.84713) | 1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.96102 HOMO: -6.80829 LUMO: -0.29933 factor:1 | 1 (-2.50429) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.00833 HOMO: -6.84094 LUMO: -0.53606 factor:1 | 1 (-1.55159) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.97325 HOMO: -6.81917 LUMO: -0.26667 factor:1 | 1 (-1.51652) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.24030 HOMO: -6.85727 LUMO: -1.20002 factor:1 | 1 (-1.78357) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18701 HOMO: -6.39468 LUMO: -1.06941 factor:1 | 1 (-2.73028) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12524.05171 HOMO: -6.00827 LUMO: -1.94017 factor:1 | 1 (-3.59498) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99575 HOMO: -6.80829 LUMO: 0.18504 factor:1 | 1 (-2.53901) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.07961 HOMO: -6.54434 LUMO: -0.95784 factor:1 | 1 (-2.62288) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.27502 HOMO: -6.45454 LUMO: -0.07347 factor:1 | 1 (-2.81828) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.82293 HOMO: -5.33887 LUMO: 1.11839 factor:1 | 1 (-2.36619) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90540 HOMO: -5.75249 LUMO: 0.70477 factor:1 | 1 (-2.44867) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.65819 HOMO: -5.64092 LUMO: 0.87076 factor:1 | 1 (-2.20146) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.93803 HOMO: -5.14295 LUMO: 1.06124 factor:1 | 1 (-2.48130) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.94670 HOMO: -5.05043 LUMO: 1.21091 factor:1 | 1 (-0.48997) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.98092 HOMO: -5.05588 LUMO: 1.02859 factor:1 | 1 (-1.52419) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.92179 HOMO: -5.76337 LUMO: 0.79457 factor:1 | 1 (-1.46506) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.12169 HOMO: -5.01506 LUMO: 1.00138 factor:1 | 1 (-1.66496) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.09069 HOMO: -4.84363 LUMO: 1.53744 factor:1 | 1 (-1.63396) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.69178 HOMO: -5.17833 LUMO: 1.45309 factor:1 | 1 (-0.23505) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.09286 HOMO: -5.13751 LUMO: 0.51157 factor:1 | -1 (0.36387) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.62977 HOMO: -5.56473 LUMO: 0.32109 factor:1 | 1 (-0.17304) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.24198 HOMO: -4.69941 LUMO: 1.14016 factor:1 | 1 (-2.78525) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14054 HOMO: -4.49260 LUMO: 1.86398 factor:1 | 1 (-2.68380) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.34397 HOMO: -4.32117 LUMO: 1.68438 factor:1 | 1 (-2.88724) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41889 HOMO: -4.44906 LUMO: 1.37690 factor:1 | 1 (-1.96216) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.94424 HOMO: -4.62049 LUMO: 1.34968 factor:1 | 1 (-1.48751) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.86000 HOMO: -4.59600 LUMO: 1.58370 factor:1 | 1 (-1.40326) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.07510 HOMO: -4.98785 LUMO: 1.46669 factor:1 | 1 (-1.61837) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.02215 HOMO: -5.06676 LUMO: 1.27349 factor:1 | 1 (-1.56542) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12520.88988 HOMO: -5.09125 LUMO: 1.13471 factor:1 | 1 (-0.43315) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.05395 HOMO: -4.84635 LUMO: 1.33608 factor:1 | 1 (-2.59722) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.14029 HOMO: -4.94431 LUMO: 1.18370 factor:1 | 1 (-2.68356) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.19355 HOMO: -4.92526 LUMO: 1.39867 factor:1 | 1 (-1.73682) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.99779 HOMO: -5.71983 LUMO: 0.60137 factor:1 | 1 (-2.54105) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.11897 HOMO: -5.10486 LUMO: 1.05580 factor:1 | 1 (-1.66223) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.18685 HOMO: -5.20282 LUMO: 1.01226 factor:1 | 1 (-2.73012) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.31968 HOMO: -4.98513 LUMO: 1.53744 factor:1 | 1 (-1.86295) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.33777 HOMO: -5.67085 LUMO: 0.17687 factor:1 | 1 (-1.88104) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.41903 HOMO: -5.87222 LUMO: 0.12517 factor:1 | 1 (-1.96229) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.09549 HOMO: -5.20826 LUMO: 0.91702 factor:1 | 1 (-0.63876) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.74199 HOMO: -5.94569 LUMO: 0.63130 factor:1 | 1 (-3.28526) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.86366 HOMO: -5.35792 LUMO: 0.91430 factor:1 | 1 (-2.40693) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.04625 HOMO: -5.36336 LUMO: 1.44220 factor:1 | 1 (-2.58952) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12522.90731 HOMO: -5.83412 LUMO: 0.71294 factor:1 | 1 (-2.45058) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12523.10924 HOMO: -4.97696 LUMO: 1.72792 factor:1 | 1 (-2.65251) | -1 | -1 |
| G: -6256.09104 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12521.01285 HOMO: -5.55929 LUMO: 0.23130 factor:1 | 1 (-0.55612) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.63887 HOMO: -5.71167 LUMO: 0.47348 factor:1 | -1 (0.23282) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.02017 HOMO: -7.31986 LUMO: -2.54699 factor:1 | -1 (1.85152) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.96118 HOMO: -5.34704 LUMO: 1.19730 factor:1 | -1 (1.91051) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.84865 HOMO: -5.45860 LUMO: 0.80818 factor:1 | -1 (1.02304) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.03949 HOMO: -5.12663 LUMO: 1.20274 factor:1 | -1 (0.83221) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60491 HOMO: -5.37153 LUMO: 1.05580 factor:1 | -1 (0.26678) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.94545 HOMO: -5.47221 LUMO: 0.97961 factor:1 | -1 (1.92624) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.22447 HOMO: -5.06948 LUMO: 1.12111 factor:1 | -1 (0.64722) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.35449 HOMO: -5.19737 LUMO: 1.25444 factor:1 | -1 (1.51720) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.47621 HOMO: -5.27901 LUMO: 1.00682 factor:1 | -1 (1.39548) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.99465 HOMO: -5.38513 LUMO: 0.49253 factor:1 | -1 (1.87704) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.57031 HOMO: -5.12390 LUMO: 1.22995 factor:1 | -1 (1.30138) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.71790 HOMO: -5.31438 LUMO: 0.70205 factor:1 | -1 (1.15379) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.33816 HOMO: -5.17561 LUMO: 1.04492 factor:1 | -1 (0.53353) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.89367 HOMO: -4.94431 LUMO: 1.52656 factor:1 | -1 (1.97802) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.38072 HOMO: -5.13751 LUMO: 0.93879 factor:1 | -1 (1.49097) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.69654 HOMO: -5.49942 LUMO: 0.97689 factor:1 | -1 (1.17515) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.62337 HOMO: -5.79058 LUMO: 0.53879 factor:1 | -1 (1.24832) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.14289 HOMO: -5.36881 LUMO: 1.56465 factor:1 | -1 (0.72880) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.51496 HOMO: -4.67492 LUMO: 1.32792 factor:1 | -1 (1.35673) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.77865 HOMO: -4.60145 LUMO: 1.19458 factor:1 | -1 (2.09305) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.98790 HOMO: -4.49260 LUMO: 1.60547 factor:1 | -1 (1.88379) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.61189 HOMO: -4.65043 LUMO: 1.34696 factor:1 | -1 (1.25981) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.86825 HOMO: -4.77560 LUMO: 1.35241 factor:1 | -1 (2.00344) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.98287 HOMO: -4.94431 LUMO: 1.17825 factor:1 | -1 (1.88882) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.49322 HOMO: -4.87084 LUMO: 1.41771 factor:1 | -1 (1.37847) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.48845 HOMO: -5.34432 LUMO: 1.16737 factor:1 | -1 (1.38324) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.41879 HOMO: -4.94975 LUMO: 1.67622 factor:1 | -1 (1.45290) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.49959 HOMO: -4.81369 LUMO: 1.14288 factor:1 | -1 (2.37210) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.58626 HOMO: -5.22459 LUMO: 0.29660 factor:1 | -1 (2.28543) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.73620 HOMO: -5.21642 LUMO: 0.37824 factor:1 | -1 (2.13550) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.77799 HOMO: -5.00417 LUMO: 1.01226 factor:1 | -1 (2.09370) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.43230 HOMO: -5.46677 LUMO: 0.10612 factor:1 | -1 (2.43939) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.84327 HOMO: -5.51303 LUMO: 0.54151 factor:1 | -1 (2.02842) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.37588 HOMO: -5.63004 LUMO: 0.17960 factor:1 | -1 (1.49581) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.43419 HOMO: -4.79193 LUMO: 1.12111 factor:1 | -1 (1.43750) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.51915 HOMO: -5.43411 LUMO: 0.45987 factor:1 | -1 (1.35254) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.23035 HOMO: -7.06135 LUMO: -2.13881 factor:1 | -1 (1.64134) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.81380 HOMO: -5.33071 LUMO: 1.14016 factor:1 | -1 (2.05789) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.45841 HOMO: -7.12394 LUMO: -0.03810 factor:1 | -1 (1.41328) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.69975 HOMO: -7.20558 LUMO: -2.50889 factor:1 | -1 (1.17194) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.45477 HOMO: -7.26816 LUMO: -2.11432 factor:1 | -1 (1.41692) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.60867 HOMO: -7.89674 LUMO: 0.31021 factor:1 | -1 (1.26302) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.27404 HOMO: -7.26544 LUMO: 0.22858 factor:1 | -1 (2.59765) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.54278 HOMO: -7.12666 LUMO: -0.02449 factor:1 | -1 (2.32891) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.69641 HOMO: -7.68722 LUMO: 0.71838 factor:1 | -1 (2.17528) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.84360 HOMO: -6.86271 LUMO: -0.96056 factor:1 | -1 (2.02809) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.70558 HOMO: -7.07496 LUMO: -1.11839 factor:1 | -1 (2.16611) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.40652 HOMO: -7.06952 LUMO: -2.08439 factor:1 | -1 (1.46517) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.87470 HOMO: -6.60965 LUMO: -2.11977 factor:1 | -1 (1.99699) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.00730 HOMO: -6.87360 LUMO: -1.85854 factor:1 | -1 (1.86439) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.38837 HOMO: -7.67089 LUMO: -0.24762 factor:1 | -1 (1.48332) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.34170 HOMO: -6.45726 LUMO: -1.86398 factor:1 | -1 (1.52999) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.42769 HOMO: -6.91713 LUMO: 0.33198 factor:1 | -1 (1.44400) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.60675 HOMO: -6.83278 LUMO: 0.26667 factor:1 | -1 (2.26494) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.81437 HOMO: -6.89264 LUMO: -1.00682 factor:1 | -1 (2.05732) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.77655 HOMO: -6.57427 LUMO: 0.22041 factor:1 | -1 (2.09514) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.05734 HOMO: -7.52123 LUMO: -0.01905 factor:1 | -1 (0.81436) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.11902 HOMO: -7.37429 LUMO: -0.08980 factor:1 | -1 (0.75267) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57136 HOMO: -7.28449 LUMO: -0.26395 factor:1 | -1 (0.30033) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.43413 HOMO: -6.79740 LUMO: -0.60954 factor:1 | -1 (0.43756) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70157 HOMO: -7.12666 LUMO: -0.60681 factor:1 | -1 (0.17013) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.90530 HOMO: -6.96611 LUMO: -0.30477 factor:1 | 1 (-0.03361) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61590 HOMO: -7.08040 LUMO: -0.31293 factor:1 | 1 (-0.74420) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.32256 HOMO: -6.78924 LUMO: -0.73743 factor:1 | 1 (-0.45087) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.32286 HOMO: -7.57293 LUMO: -1.11295 factor:1 | -1 (0.54883) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.32844 HOMO: -7.15932 LUMO: -0.23130 factor:1 | -1 (0.54325) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14242 HOMO: -7.48585 LUMO: -0.10068 factor:1 | 1 (-0.27073) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.99322 HOMO: -7.17020 LUMO: -0.26123 factor:1 | 1 (-0.12153) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.22207 HOMO: -7.43143 LUMO: -0.16055 factor:1 | -1 (0.64962) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.33846 HOMO: -7.14843 LUMO: -0.10612 factor:1 | -1 (0.53323) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.19110 HOMO: -6.95523 LUMO: -0.22585 factor:1 | 1 (-0.31941) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17722 HOMO: -7.06680 LUMO: -0.51974 factor:1 | 1 (-0.30553) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.02557 HOMO: -6.80829 LUMO: -0.64763 factor:1 | 1 (-0.15388) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.26425 HOMO: -7.13210 LUMO: -0.48164 factor:1 | -1 (0.60744) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.19676 HOMO: -7.16204 LUMO: -0.45715 factor:1 | 1 (-0.32507) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.94447 HOMO: -7.15115 LUMO: -0.43266 factor:1 | 1 (-1.07278) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.17552 HOMO: -7.15932 LUMO: -2.52794 factor:1 | 1 (-1.30383) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.06907 HOMO: -7.21102 LUMO: -2.65311 factor:1 | 1 (-1.19738) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.90021 HOMO: -6.57427 LUMO: -2.78645 factor:1 | 1 (-0.02852) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01561 HOMO: -6.40828 LUMO: -3.23815 factor:1 | 1 (-0.14392) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.39316 HOMO: -7.71987 LUMO: -0.20953 factor:1 | 1 (-1.52147) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.05207 HOMO: -7.47769 LUMO: -0.43810 factor:1 | 1 (-1.18038) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.34079 HOMO: -6.68040 LUMO: -2.22589 factor:1 | 1 (-0.46910) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.32166 HOMO: -6.92802 LUMO: -1.99187 factor:1 | 1 (-0.44997) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.29031 HOMO: -7.73620 LUMO: 0.01633 factor:1 | 1 (-0.41862) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.64528 HOMO: -7.28721 LUMO: -0.18504 factor:1 | 1 (-0.77359) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.64387 HOMO: -7.49674 LUMO: -0.19864 factor:1 | 1 (-0.77218) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.63356 HOMO: -7.10489 LUMO: -2.56331 factor:1 | 1 (-0.76186) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.56169 HOMO: -7.36612 LUMO: 0.16055 factor:1 | 1 (-0.69000) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.75075 HOMO: -7.67633 LUMO: 0.33198 factor:1 | 1 (-0.87906) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.72543 HOMO: -7.07768 LUMO: -0.27483 factor:1 | -1 (0.14626) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.08680 HOMO: -7.32531 LUMO: 0.05442 factor:1 | 1 (-0.21511) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.07806 HOMO: -6.79740 LUMO: -1.21635 factor:1 | 1 (-0.20637) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61802 HOMO: -7.14027 LUMO: 0.12517 factor:1 | 1 (-0.74633) | 1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.39189 HOMO: -7.17292 LUMO: 0.16871 factor:1 | 1 (-0.52020) | 1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.46705 HOMO: -7.08312 LUMO: -1.38778 factor:1 | 1 (-0.59536) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50338 HOMO: -6.75387 LUMO: -1.88031 factor:1 | 1 (-0.63169) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.37259 HOMO: -7.07768 LUMO: -1.25717 factor:1 | -1 (1.49910) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.34846 HOMO: -6.46543 LUMO: -1.14016 factor:1 | 1 (-0.47677) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.27950 HOMO: -7.37973 LUMO: -0.45987 factor:1 | 1 (-1.40781) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.08262 HOMO: -7.46408 LUMO: 0.03265 factor:1 | 1 (-1.21093) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30188 HOMO: -7.96477 LUMO: -0.19864 factor:1 | 1 (-0.43018) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.99265 HOMO: -6.93890 LUMO: -1.11839 factor:1 | 1 (-0.12095) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85828 HOMO: -7.06408 LUMO: -1.08846 factor:1 | -1 (0.01342) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.70827 HOMO: -7.14027 LUMO: -0.33470 factor:1 | -1 (1.16342) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.33518 HOMO: -7.38245 LUMO: 0.10885 factor:1 | 1 (-0.46349) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.51894 HOMO: -7.59470 LUMO: -1.21363 factor:1 | 1 (-0.64725) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.62153 HOMO: -7.23279 LUMO: -1.23812 factor:1 | 1 (-0.74984) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.23651 HOMO: -6.90897 LUMO: 0.23402 factor:1 | 1 (-1.36481) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.95772 HOMO: -7.36340 LUMO: -0.17143 factor:1 | 1 (-1.08603) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.34931 HOMO: -6.61781 LUMO: -0.01361 factor:1 | 1 (-0.47761) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36041 HOMO: -6.80013 LUMO: 0.38368 factor:1 | 1 (-0.48872) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46777 HOMO: -6.72121 LUMO: -0.95512 factor:1 | -1 (0.40393) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.24041 HOMO: -6.24773 LUMO: -0.69933 factor:1 | 1 (-0.36871) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14253 HOMO: -6.56883 LUMO: 0.14694 factor:1 | 1 (-0.27083) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50823 HOMO: -6.51441 LUMO: -1.27621 factor:1 | -1 (0.36346) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.40899 HOMO: -6.91986 LUMO: -1.16737 factor:1 | -1 (0.46270) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.57270 HOMO: -6.17971 LUMO: -0.65307 factor:1 | 1 (-1.70101) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.97362 HOMO: -7.22462 LUMO: 0.04354 factor:1 | 1 (-1.10193) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.83024 HOMO: -7.16204 LUMO: -0.23674 factor:1 | 1 (-0.95855) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.81624 HOMO: -6.81645 LUMO: -0.19320 factor:1 | 1 (-1.94455) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.40586 HOMO: -6.69400 LUMO: 0.04082 factor:1 | -1 (0.46583) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20250 HOMO: -6.63141 LUMO: -0.22858 factor:1 | 1 (-0.33081) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60290 HOMO: -6.92258 LUMO: -1.11295 factor:1 | -1 (0.26879) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.39741 HOMO: -6.60148 LUMO: -1.13744 factor:1 | 1 (-0.52572) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.28195 HOMO: -6.78108 LUMO: -0.82450 factor:1 | 1 (-1.41026) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.46345 HOMO: -7.05591 LUMO: -0.97145 factor:1 | 1 (-1.59176) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.54953 HOMO: -6.65318 LUMO: -1.26261 factor:1 | 1 (-0.67784) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.28562 HOMO: -6.98244 LUMO: -0.98233 factor:1 | 1 (-1.41393) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.60164 HOMO: -7.11850 LUMO: -0.99594 factor:1 | 1 (-0.72995) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.41758 HOMO: -6.64230 LUMO: -0.93879 factor:1 | 1 (-0.54589) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.19841 HOMO: -6.62053 LUMO: -1.22451 factor:1 | 1 (-1.32672) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.83965 HOMO: -7.02598 LUMO: -0.85172 factor:1 | 1 (-0.96796) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.54482 HOMO: -7.06680 LUMO: -0.89253 factor:1 | 1 (-0.67313) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.94965 HOMO: -7.17292 LUMO: 0.00272 factor:1 | 1 (-0.07796) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.93248 HOMO: -7.03142 LUMO: -0.35103 factor:1 | 1 (-0.06079) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.04886 HOMO: -6.96884 LUMO: -0.09796 factor:1 | 1 (-0.17717) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05474 HOMO: -6.56339 LUMO: -0.99322 factor:1 | 1 (-0.18305) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.93931 HOMO: -7.08857 LUMO: -0.17687 factor:1 | 1 (-0.06762) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.19093 HOMO: -7.05863 LUMO: -0.22041 factor:1 | 1 (-1.31924) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.51129 HOMO: -7.15115 LUMO: -0.17960 factor:1 | 1 (-0.63960) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.51423 HOMO: -6.67495 LUMO: -0.96600 factor:1 | 1 (-0.64254) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69974 HOMO: -6.74026 LUMO: -1.79867 factor:1 | -1 (0.17195) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.04418 HOMO: -6.73482 LUMO: -1.78235 factor:1 | 1 (-1.17248) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30291 HOMO: -6.09807 LUMO: 0.16871 factor:1 | 1 (-0.43122) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.92093 HOMO: -6.72393 LUMO: 0.27211 factor:1 | 1 (-1.04924) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.20886 HOMO: -6.40556 LUMO: -0.04354 factor:1 | 1 (-1.33717) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.36843 HOMO: -6.56883 LUMO: 0.22041 factor:1 | 1 (-1.49674) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.76123 HOMO: -7.22462 LUMO: 0.15783 factor:1 | 1 (-0.88954) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87215 HOMO: -6.83550 LUMO: 0.19320 factor:1 | 1 (-0.00046) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.87800 HOMO: -7.26816 LUMO: -0.07619 factor:1 | 1 (-1.00630) | 1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.79724 HOMO: -7.13483 LUMO: 0.33198 factor:1 | -1 (0.07445) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.73715 HOMO: -6.58243 LUMO: -0.26395 factor:1 | 1 (-0.86546) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.76556 HOMO: -7.38517 LUMO: 0.17143 factor:1 | 1 (-0.89387) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.84975 HOMO: -6.80013 LUMO: 0.25851 factor:1 | 1 (-0.97806) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69588 HOMO: -6.96611 LUMO: 0.11429 factor:1 | -1 (0.17581) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.76787 HOMO: -6.51713 LUMO: -1.14560 factor:1 | 1 (-0.89618) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.51984 HOMO: -7.15387 LUMO: -0.35647 factor:1 | 1 (-0.64815) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.53419 HOMO: -5.26540 LUMO: 1.26805 factor:1 | -1 (0.33750) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.00905 HOMO: -6.76475 LUMO: -0.16327 factor:1 | 1 (-0.13736) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.00541 HOMO: -6.55250 LUMO: -0.71838 factor:1 | 1 (-0.13372) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.38572 HOMO: -6.76203 LUMO: -1.08301 factor:1 | -1 (0.48597) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.14954 HOMO: -7.14027 LUMO: -0.01633 factor:1 | -1 (1.72215) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.02753 HOMO: -6.94979 LUMO: -0.93879 factor:1 | 1 (-0.15584) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88380 HOMO: -6.74842 LUMO: 0.31293 factor:1 | 1 (-0.01211) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.32526 HOMO: -6.43821 LUMO: 0.05987 factor:1 | -1 (0.54643) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01548 HOMO: -6.60420 LUMO: 0.22585 factor:1 | 1 (-0.14378) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.78048 HOMO: -6.43821 LUMO: 0.05987 factor:1 | -1 (0.09121) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76238 HOMO: -6.34570 LUMO: 1.43948 factor:1 | -1 (0.10931) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.13011 HOMO: -6.03004 LUMO: 1.21363 factor:1 | 1 (-1.25842) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.24772 HOMO: -6.68040 LUMO: -0.92247 factor:1 | 1 (-0.37603) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.04143 HOMO: -6.92530 LUMO: -0.31293 factor:1 | 1 (-1.16974) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.98486 HOMO: -6.94979 LUMO: -0.19864 factor:1 | 1 (-0.11317) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91267 HOMO: -6.80829 LUMO: -0.30477 factor:1 | 1 (-0.04098) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.68166 HOMO: -7.22734 LUMO: -1.02859 factor:1 | 1 (-1.80997) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.12992 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-1.25823) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.64881 HOMO: -7.27088 LUMO: -0.78097 factor:1 | 1 (-1.77712) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.10682 HOMO: -7.29809 LUMO: -0.97145 factor:1 | 1 (-1.23512) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.58945 HOMO: -7.18925 LUMO: -0.94696 factor:1 | 1 (-0.71775) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.58980 HOMO: -7.33891 LUMO: -0.96873 factor:1 | 1 (-0.71811) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.08772 HOMO: -7.36068 LUMO: -0.28028 factor:1 | 1 (-0.21603) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.69851 HOMO: -7.10761 LUMO: -1.14832 factor:1 | 1 (-0.82682) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.86062 HOMO: -6.94707 LUMO: -0.65307 factor:1 | -1 (0.01108) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.84051 HOMO: -6.91713 LUMO: -1.81228 factor:1 | -1 (0.03118) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.09793 HOMO: -6.78652 LUMO: -2.01636 factor:1 | 1 (-0.22624) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.97599 HOMO: -6.52801 LUMO: -1.17553 factor:1 | 1 (-0.10430) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89485 HOMO: -7.54844 LUMO: -1.18642 factor:1 | 1 (-0.02316) | 1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06778 HOMO: -7.52939 LUMO: -1.23812 factor:1 | 1 (-0.19609) | 1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01877 HOMO: -7.94572 LUMO: -0.81634 factor:1 | 1 (-0.14708) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76984 HOMO: -7.55932 LUMO: -0.86260 factor:1 | -1 (0.10185) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.92092 HOMO: -7.72259 LUMO: -1.39050 factor:1 | 1 (-0.04923) | 1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.63718 HOMO: -7.11850 LUMO: -1.01498 factor:1 | -1 (0.23451) | 1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77204 HOMO: -7.09673 LUMO: -1.00954 factor:1 | -1 (0.09965) | 1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.35545 HOMO: -6.06270 LUMO: 0.16327 factor:1 | -1 (1.51625) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.85269 HOMO: -5.71167 LUMO: 0.70477 factor:1 | 1 (-0.98100) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.87609 HOMO: -5.38241 LUMO: 0.86260 factor:1 | 1 (-1.00440) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.77575 HOMO: -5.67357 LUMO: 1.27621 factor:1 | -1 (1.09594) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.20256 HOMO: -7.56204 LUMO: -0.68573 factor:1 | -1 (0.66913) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.25694 HOMO: -5.57833 LUMO: 1.13199 factor:1 | 1 (-1.38525) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.35542 HOMO: -7.58653 LUMO: -0.66124 factor:1 | 1 (-1.48373) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.85875 HOMO: -7.91851 LUMO: -1.10206 factor:1 | 1 (-1.98706) | 1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.56982 HOMO: -6.48992 LUMO: -1.00138 factor:1 | 1 (-1.69813) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.27461 HOMO: -7.09673 LUMO: -0.45171 factor:1 | 1 (-0.40292) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88415 HOMO: -6.63686 LUMO: 0.09252 factor:1 | 1 (-0.01246) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.83476 HOMO: -6.84366 LUMO: -0.14422 factor:1 | -1 (0.03693) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.31880 HOMO: -6.93074 LUMO: 0.04354 factor:1 | 1 (-0.44711) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87308 HOMO: -6.90353 LUMO: -0.19864 factor:1 | 1 (-0.00139) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81719 HOMO: -6.59876 LUMO: -0.10068 factor:1 | -1 (0.05450) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.95030 HOMO: -6.74570 LUMO: -0.44627 factor:1 | 1 (-0.07861) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61810 HOMO: -6.60148 LUMO: -0.61770 factor:1 | 1 (-0.74641) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.74714 HOMO: -6.55794 LUMO: -1.06941 factor:1 | -1 (0.12455) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.44647 HOMO: -7.12666 LUMO: -0.11973 factor:1 | 1 (-1.57478) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.30192 HOMO: -7.21646 LUMO: -0.50069 factor:1 | 1 (-1.43023) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.81203 HOMO: -7.27632 LUMO: -1.00682 factor:1 | 1 (-0.94034) | 1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96301 HOMO: -6.74298 LUMO: 0.04354 factor:1 | 1 (-0.09132) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.86390 HOMO: -6.37291 LUMO: 0.14150 factor:1 | 1 (-0.99221) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.20078 HOMO: -5.61371 LUMO: 1.28438 factor:1 | 1 (-1.32909) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.52580 HOMO: -5.52119 LUMO: 0.99866 factor:1 | 1 (-0.65411) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.54095 HOMO: -6.51985 LUMO: -0.10885 factor:1 | 1 (-0.66926) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.91030 HOMO: -5.61371 LUMO: 0.77280 factor:1 | 1 (-1.03860) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.91674 HOMO: -5.58922 LUMO: 0.24490 factor:1 | 1 (-1.04505) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.98486 HOMO: -6.32665 LUMO: -0.57144 factor:1 | 1 (-0.11317) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.29735 HOMO: -6.29127 LUMO: -0.93607 factor:1 | 1 (-1.42566) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.57720 HOMO: -5.49670 LUMO: 0.27211 factor:1 | 1 (-0.70551) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.52457 HOMO: -5.68990 LUMO: 0.24218 factor:1 | 1 (-0.65288) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.86817 HOMO: -5.68174 LUMO: 0.69933 factor:1 | 1 (-0.99648) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.42028 HOMO: -5.28173 LUMO: 1.00954 factor:1 | -1 (0.45141) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.51561 HOMO: -5.94025 LUMO: 0.73471 factor:1 | -1 (1.35608) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.07045 HOMO: -5.65725 LUMO: 1.28710 factor:1 | -1 (0.80124) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.13884 HOMO: -5.41507 LUMO: 0.87076 factor:1 | 1 (-1.26715) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.15300 HOMO: -5.96474 LUMO: 0.29660 factor:1 | 1 (-0.28131) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.02703 HOMO: -7.00421 LUMO: 0.08708 factor:1 | 1 (-1.15534) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.13491 HOMO: -5.40418 LUMO: 0.90070 factor:1 | 1 (-0.26322) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.48446 HOMO: -7.00421 LUMO: -0.30477 factor:1 | 1 (-0.61277) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.61857 HOMO: -5.85861 LUMO: 0.74015 factor:1 | -1 (0.25312) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.75225 HOMO: -5.71439 LUMO: 0.26395 factor:1 | 1 (-0.88056) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.53881 HOMO: -7.13755 LUMO: -0.78369 factor:1 | 1 (-0.66711) | 1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.66946 HOMO: -7.31442 LUMO: -0.98233 factor:1 | -1 (0.20224) | 1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.39054 HOMO: -7.25728 LUMO: -1.00410 factor:1 | -1 (0.48115) | 1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.98159 HOMO: -7.48585 LUMO: -0.83811 factor:1 | 1 (-1.10990) | 1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87452 HOMO: -7.24911 LUMO: -0.77280 factor:1 | 1 (-0.00283) | 1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36873 HOMO: -7.55116 LUMO: -1.19730 factor:1 | 1 (-0.49704) | 1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80481 HOMO: -5.76881 LUMO: 0.28028 factor:1 | -1 (0.06689) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60643 HOMO: -5.77153 LUMO: -0.26939 factor:1 | -1 (0.26526) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.65695 HOMO: -5.82868 LUMO: 0.36735 factor:1 | -1 (1.21474) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79799 HOMO: -5.83140 LUMO: -0.17960 factor:1 | 1 (-0.92630) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.08130 HOMO: -6.28855 LUMO: 0.01088 factor:1 | 1 (-0.20961) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.63021 HOMO: -6.31576 LUMO: 0.25307 factor:1 | 1 (-0.75852) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.38437 HOMO: -7.06408 LUMO: -2.76196 factor:1 | -1 (1.48732) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.10922 HOMO: -5.95657 LUMO: 0.37552 factor:1 | 1 (-0.23753) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14674 HOMO: -6.61781 LUMO: 0.02721 factor:1 | 1 (-0.27505) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.17071 HOMO: -6.26678 LUMO: -0.66668 factor:1 | -1 (1.70098) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.93507 HOMO: -6.00011 LUMO: -0.13334 factor:1 | 1 (-0.06338) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23368 HOMO: -5.60555 LUMO: 0.67484 factor:1 | 1 (-0.36199) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17439 HOMO: -5.79875 LUMO: 0.99049 factor:1 | 1 (-0.30270) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.16519 HOMO: -5.97834 LUMO: 0.48436 factor:1 | 1 (-0.29350) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.67919 HOMO: -5.82868 LUMO: 0.91974 factor:1 | -1 (2.19250) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57460 HOMO: -5.86677 LUMO: 0.99594 factor:1 | -1 (0.29709) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.61140 HOMO: -5.70079 LUMO: 0.48980 factor:1 | -1 (1.26030) | -1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.90023 HOMO: -7.39605 LUMO: -1.02315 factor:1 | -1 (1.97146) | 1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88843 HOMO: -7.22734 LUMO: -1.12927 factor:1 | 1 (-0.01674) | 1 | -1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.19913 HOMO: -7.58926 LUMO: -0.65035 factor:1 | 1 (-0.32743) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.75618 HOMO: -7.43959 LUMO: -0.75648 factor:1 | -1 (0.11551) | 1 | 1 |
| G: -6695.50600 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.92394 HOMO: -7.55388 LUMO: -1.15104 factor:1 | 1 (-0.05225) | 1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.42717 HOMO: -6.74570 LUMO: -2.85447 factor:1 | -1 (0.44453) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.50350 HOMO: -7.35524 LUMO: -1.25444 factor:1 | -1 (1.36819) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.55722 HOMO: -6.81645 LUMO: -1.20819 factor:1 | -1 (1.31447) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.22442 HOMO: -6.99605 LUMO: -1.62996 factor:1 | -1 (1.64727) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.31417 HOMO: -6.88992 LUMO: -0.47620 factor:1 | -1 (1.55753) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52616 HOMO: -7.22190 LUMO: -0.01905 factor:1 | -1 (0.34553) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.67061 HOMO: -6.77836 LUMO: -0.82995 factor:1 | -1 (1.20108) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.37283 HOMO: -6.48447 LUMO: -0.95512 factor:1 | -1 (1.49886) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.92392 HOMO: -7.81239 LUMO: 1.22179 factor:1 | -1 (0.94777) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.71513 HOMO: -7.36612 LUMO: 0.19320 factor:1 | 1 (-0.84344) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05575 HOMO: -7.24095 LUMO: 0.33470 factor:1 | 1 (-0.18406) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.81818 HOMO: -7.15932 LUMO: -2.24222 factor:1 | 1 (-0.94649) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.29227 HOMO: -6.88992 LUMO: -2.69937 factor:1 | 1 (-0.42058) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.08797 HOMO: -6.97428 LUMO: -0.98233 factor:1 | 1 (-0.21628) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.19039 HOMO: -7.17564 LUMO: -0.93879 factor:1 | 1 (-0.31870) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.74292 HOMO: -6.81645 LUMO: -1.14288 factor:1 | 1 (-0.87123) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14408 HOMO: -6.83006 LUMO: -0.63403 factor:1 | 1 (-0.27239) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14500 HOMO: -7.17292 LUMO: -1.07213 factor:1 | 1 (-0.27331) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80105 HOMO: -7.53755 LUMO: 0.15510 factor:1 | -1 (0.07064) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.92046 HOMO: -6.50080 LUMO: -0.51702 factor:1 | -1 (0.95123) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.03678 HOMO: -6.72665 LUMO: -0.80001 factor:1 | 1 (-0.16509) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81645 HOMO: -6.72665 LUMO: 1.68711 factor:1 | -1 (0.05524) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11678 HOMO: -7.11850 LUMO: -0.75103 factor:1 | 1 (-0.24509) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.27583 HOMO: -6.87087 LUMO: -0.85988 factor:1 | 1 (-0.40414) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11510 HOMO: -7.08857 LUMO: -0.89798 factor:1 | 1 (-0.24341) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.07253 HOMO: -6.71305 LUMO: -0.85444 factor:1 | -1 (1.79916) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.47333 HOMO: -6.59332 LUMO: -0.60137 factor:1 | 1 (-0.60164) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.31834 HOMO: -7.28993 LUMO: 0.03265 factor:1 | 1 (-0.44665) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81762 HOMO: -7.32258 LUMO: 0.13878 factor:1 | -1 (0.05407) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.04264 HOMO: -7.28993 LUMO: 0.11429 factor:1 | -1 (0.82905) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.27992 HOMO: -6.86271 LUMO: -1.03947 factor:1 | 1 (-0.40823) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.02307 HOMO: -6.55794 LUMO: -0.84900 factor:1 | 1 (-0.15138) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01436 HOMO: -7.03686 LUMO: 0.11429 factor:1 | 1 (-0.14267) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.10908 HOMO: -7.06952 LUMO: -0.96056 factor:1 | 1 (-0.23739) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62080 HOMO: -6.90897 LUMO: -0.99866 factor:1 | -1 (0.25089) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.99608 HOMO: -7.00693 LUMO: -0.83539 factor:1 | -1 (0.87561) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.32343 HOMO: -6.74298 LUMO: -0.85172 factor:1 | 1 (-0.45174) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45862 HOMO: -6.83822 LUMO: -1.07213 factor:1 | -1 (0.41307) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23709 HOMO: -7.21918 LUMO: -1.55377 factor:1 | 1 (-0.36539) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57179 HOMO: -6.84094 LUMO: -1.09934 factor:1 | -1 (0.29990) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62692 HOMO: -7.09129 LUMO: -0.85988 factor:1 | -1 (0.24477) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.66762 HOMO: -6.57971 LUMO: -2.27215 factor:1 | 1 (-0.79593) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.33769 HOMO: -6.81373 LUMO: -1.86942 factor:1 | 1 (-0.46599) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.65840 HOMO: -6.59060 LUMO: -2.30480 factor:1 | 1 (-0.78671) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.84625 HOMO: -6.72938 LUMO: -1.23540 factor:1 | -1 (0.02544) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.51625 HOMO: -6.94707 LUMO: -2.62318 factor:1 | 1 (-0.64456) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79691 HOMO: -7.28177 LUMO: -0.09796 factor:1 | 1 (-0.92521) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05637 HOMO: -6.80013 LUMO: -0.79729 factor:1 | 1 (-0.18468) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.95108 HOMO: -7.26544 LUMO: 0.12789 factor:1 | 1 (-1.07939) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.98037 HOMO: -6.51713 LUMO: -0.49253 factor:1 | 1 (-0.10868) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.92230 HOMO: -6.68856 LUMO: -0.77280 factor:1 | 1 (-1.05060) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.69157 HOMO: -6.41100 LUMO: -0.70750 factor:1 | 1 (-0.81988) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87253 HOMO: -7.56204 LUMO: 0.22041 factor:1 | 1 (-0.00084) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.53285 HOMO: -6.68312 LUMO: 1.30343 factor:1 | 1 (-0.66116) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01246 HOMO: -7.24367 LUMO: 0.17415 factor:1 | 1 (-0.14076) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.58158 HOMO: -7.52395 LUMO: 1.16737 factor:1 | 1 (-0.70989) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.74490 HOMO: -6.89264 LUMO: 0.23130 factor:1 | 1 (-0.87321) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.63998 HOMO: -7.21102 LUMO: 0.19048 factor:1 | 1 (-0.76829) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.26777 HOMO: -7.08312 LUMO: 0.25034 factor:1 | -1 (1.60392) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.63481 HOMO: -6.49536 LUMO: -0.65852 factor:1 | 1 (-0.76312) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64986 HOMO: -6.85455 LUMO: 0.13606 factor:1 | -1 (0.22183) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06514 HOMO: -7.10217 LUMO: 0.35919 factor:1 | 1 (-0.19345) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.72399 HOMO: -7.77429 LUMO: 1.19186 factor:1 | -1 (0.14770) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11714 HOMO: -6.57427 LUMO: -0.50069 factor:1 | 1 (-0.24545) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.13058 HOMO: -7.36340 LUMO: 0.10068 factor:1 | 1 (-0.25889) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96761 HOMO: -7.28177 LUMO: 0.15238 factor:1 | 1 (-0.09592) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06587 HOMO: -6.86543 LUMO: -0.84355 factor:1 | 1 (-0.19418) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.28364 HOMO: -6.55794 LUMO: 1.39594 factor:1 | 1 (-0.41195) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.22283 HOMO: -6.26134 LUMO: 1.53744 factor:1 | 1 (-0.35114) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30511 HOMO: -5.97562 LUMO: 1.42316 factor:1 | 1 (-0.43342) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.37377 HOMO: -6.65046 LUMO: 1.44492 factor:1 | 1 (-0.50208) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89798 HOMO: -6.92258 LUMO: 0.17415 factor:1 | 1 (-0.02629) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.44737 HOMO: -7.40966 LUMO: 0.19592 factor:1 | 1 (-0.57568) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.29942 HOMO: -7.17564 LUMO: 0.16871 factor:1 | -1 (1.57227) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89858 HOMO: -7.46953 LUMO: 0.22313 factor:1 | 1 (-0.02688) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52850 HOMO: -6.13345 LUMO: 1.85854 factor:1 | -1 (0.34319) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.60209 HOMO: -6.99333 LUMO: -1.65717 factor:1 | -1 (1.26960) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.37032 HOMO: -6.93074 LUMO: -1.79323 factor:1 | -1 (0.50137) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88788 HOMO: -6.87904 LUMO: -1.79323 factor:1 | 1 (-0.01619) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.38795 HOMO: -6.84094 LUMO: 0.66940 factor:1 | 1 (-0.51625) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.37668 HOMO: -7.13210 LUMO: -1.17553 factor:1 | 1 (-0.50499) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.67181 HOMO: -6.52801 LUMO: -2.23678 factor:1 | 1 (-0.80012) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85602 HOMO: -6.81917 LUMO: -1.86398 factor:1 | -1 (0.01567) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.72486 HOMO: -7.30626 LUMO: -1.66806 factor:1 | -1 (0.14683) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.78096 HOMO: -6.98516 LUMO: -1.40683 factor:1 | 1 (-0.90927) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.86829 HOMO: -6.95523 LUMO: -0.97145 factor:1 | -1 (0.00340) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.64338 HOMO: -6.83278 LUMO: -2.68848 factor:1 | 1 (-0.77169) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59332 HOMO: -7.25456 LUMO: -2.97420 factor:1 | -1 (0.27837) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.65383 HOMO: -6.80557 LUMO: -2.65039 factor:1 | 1 (-0.78214) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.12617 HOMO: -7.10489 LUMO: 0.77008 factor:1 | 1 (-0.25448) | 1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.99953 HOMO: -7.28993 LUMO: -1.06124 factor:1 | 1 (-0.12784) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.34129 HOMO: -7.11578 LUMO: -1.10206 factor:1 | -1 (0.53040) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.00239 HOMO: -6.91713 LUMO: -1.36329 factor:1 | 1 (-0.13070) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.44245 HOMO: -7.07224 LUMO: 0.51974 factor:1 | 1 (-0.57076) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.46150 HOMO: -7.22734 LUMO: -0.93335 factor:1 | 1 (-0.58981) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.68420 HOMO: -7.19469 LUMO: -0.96600 factor:1 | 1 (-0.81250) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.42294 HOMO: -6.93890 LUMO: -0.66940 factor:1 | 1 (-0.55125) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.43369 HOMO: -7.09673 LUMO: -1.05852 factor:1 | 1 (-0.56200) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.70158 HOMO: -7.19197 LUMO: -2.26943 factor:1 | 1 (-0.82989) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.46052 HOMO: -6.90081 LUMO: -2.64767 factor:1 | 1 (-0.58883) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64154 HOMO: -6.93890 LUMO: -2.65039 factor:1 | -1 (0.23015) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20498 HOMO: -6.80013 LUMO: -2.54154 factor:1 | 1 (-0.33329) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.31916 HOMO: -6.68040 LUMO: -0.89798 factor:1 | -1 (0.55253) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.65620 HOMO: -7.01782 LUMO: -1.09662 factor:1 | -1 (0.21549) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.68316 HOMO: -6.58516 LUMO: -0.83539 factor:1 | 1 (-0.81147) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.87035 HOMO: -7.46953 LUMO: 0.06259 factor:1 | 1 (-0.99866) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81776 HOMO: -6.96884 LUMO: -0.99866 factor:1 | -1 (0.05393) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46567 HOMO: -7.29809 LUMO: -0.19320 factor:1 | -1 (0.40602) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.11546 HOMO: -6.86271 LUMO: 0.04082 factor:1 | -1 (0.75623) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.47336 HOMO: -6.36746 LUMO: -1.02587 factor:1 | 1 (-0.60167) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06737 HOMO: -7.15659 LUMO: -1.25989 factor:1 | 1 (-0.19568) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.73215 HOMO: -6.69128 LUMO: -0.59865 factor:1 | -1 (0.13954) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58045 HOMO: -7.09129 LUMO: -1.08573 factor:1 | -1 (0.29124) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.13409 HOMO: -6.64502 LUMO: -0.66396 factor:1 | 1 (-0.26240) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.21979 HOMO: -6.93346 LUMO: -0.87349 factor:1 | -1 (0.65190) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23001 HOMO: -6.77019 LUMO: -0.87349 factor:1 | 1 (-0.35832) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91504 HOMO: -6.59060 LUMO: -0.82995 factor:1 | 1 (-0.04335) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60785 HOMO: -7.17564 LUMO: -1.08846 factor:1 | -1 (0.26384) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50901 HOMO: -7.27088 LUMO: -1.18642 factor:1 | 1 (-0.63732) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.43694 HOMO: -7.06680 LUMO: -1.13199 factor:1 | -1 (1.43475) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64148 HOMO: -7.21918 LUMO: -1.03947 factor:1 | -1 (0.23021) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06745 HOMO: -7.26000 LUMO: -0.11973 factor:1 | 1 (-0.19576) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.52240 HOMO: -6.77564 LUMO: 0.23402 factor:1 | 1 (-0.65071) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.99615 HOMO: -7.07224 LUMO: -0.75648 factor:1 | 1 (-1.12446) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.96638 HOMO: -7.45048 LUMO: 0.18232 factor:1 | 1 (-1.09469) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.67364 HOMO: -7.48313 LUMO: 0.15238 factor:1 | 1 (-0.80195) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.03794 HOMO: -6.60692 LUMO: -0.50885 factor:1 | 1 (-1.16625) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.34053 HOMO: -6.62869 LUMO: -0.60954 factor:1 | 1 (-1.46884) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.76482 HOMO: -7.40422 LUMO: -1.28982 factor:1 | 1 (-0.89313) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.23849 HOMO: -6.75114 LUMO: -1.23268 factor:1 | 1 (-1.36680) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.63066 HOMO: -6.84638 LUMO: -0.73199 factor:1 | 1 (-1.75897) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.26897 HOMO: -6.79196 LUMO: -1.43676 factor:1 | 1 (-1.39728) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76568 HOMO: -7.00965 LUMO: -1.37690 factor:1 | -1 (0.10602) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.55027 HOMO: -6.97972 LUMO: -1.58098 factor:1 | -1 (0.32142) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58080 HOMO: -6.91169 LUMO: -1.48574 factor:1 | -1 (0.29089) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.98884 HOMO: -6.90081 LUMO: -1.30343 factor:1 | -1 (0.88285) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79388 HOMO: -6.78652 LUMO: -1.51840 factor:1 | 1 (-0.92219) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89009 HOMO: -6.84638 LUMO: -1.15104 factor:1 | 1 (-0.01839) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.38101 HOMO: -6.61237 LUMO: -0.89798 factor:1 | 1 (-0.50932) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.28739 HOMO: -7.16204 LUMO: -1.30070 factor:1 | 1 (-1.41570) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.73369 HOMO: -7.32803 LUMO: 0.14694 factor:1 | 1 (-0.86200) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.37131 HOMO: -6.99877 LUMO: -0.87621 factor:1 | 1 (-1.49962) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.40278 HOMO: -6.99877 LUMO: -0.97145 factor:1 | 1 (-0.53108) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.78635 HOMO: -7.08040 LUMO: -1.09662 factor:1 | 1 (-0.91466) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.00843 HOMO: -6.90897 LUMO: -1.14016 factor:1 | 1 (-0.13674) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85730 HOMO: -6.68312 LUMO: -0.74831 factor:1 | -1 (0.01439) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.74374 HOMO: -6.99061 LUMO: -0.86804 factor:1 | -1 (0.12795) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.49966 HOMO: -7.10761 LUMO: -1.18642 factor:1 | -1 (0.37203) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52156 HOMO: -6.79196 LUMO: -0.71294 factor:1 | -1 (0.35013) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69710 HOMO: -6.86271 LUMO: -0.81362 factor:1 | -1 (0.17459) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.56265 HOMO: -7.01510 LUMO: -0.99322 factor:1 | -1 (0.30904) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.08860 HOMO: -6.88720 LUMO: -0.87893 factor:1 | -1 (0.78309) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91175 HOMO: -6.88448 LUMO: 0.22041 factor:1 | 1 (-0.04006) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.04214 HOMO: -7.55932 LUMO: 1.12111 factor:1 | 1 (-0.17045) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70782 HOMO: -6.46815 LUMO: -0.86260 factor:1 | -1 (0.16387) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52477 HOMO: -7.13755 LUMO: 0.23130 factor:1 | -1 (0.34692) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.56113 HOMO: -6.78924 LUMO: 1.51023 factor:1 | -1 (0.31056) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.96860 HOMO: -6.48992 LUMO: 1.74969 factor:1 | -1 (0.90309) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.39513 HOMO: -6.78380 LUMO: 1.81500 factor:1 | 1 (-0.52344) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30302 HOMO: -6.49536 LUMO: 1.70615 factor:1 | 1 (-0.43133) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.71576 HOMO: -6.38651 LUMO: 1.44492 factor:1 | 1 (-0.84407) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.99762 HOMO: -6.83822 LUMO: 1.38234 factor:1 | 1 (-1.12593) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.71475 HOMO: -6.01644 LUMO: 1.20274 factor:1 | 1 (-1.84305) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.00222 HOMO: -6.18243 LUMO: 1.77962 factor:1 | 1 (-1.13052) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.56903 HOMO: -6.81917 LUMO: -1.01771 factor:1 | 1 (-1.69734) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14680 HOMO: -6.61237 LUMO: -0.91702 factor:1 | 1 (-0.27511) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.72518 HOMO: -6.84094 LUMO: -0.84900 factor:1 | 1 (-0.85349) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.71633 HOMO: -6.81917 LUMO: -1.01771 factor:1 | 1 (-0.84464) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50887 HOMO: -7.86953 LUMO: 1.16737 factor:1 | 1 (-0.63718) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79271 HOMO: -7.40694 LUMO: 0.11429 factor:1 | 1 (-0.92102) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.18244 HOMO: -6.70489 LUMO: -0.65035 factor:1 | 1 (-1.31075) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.10341 HOMO: -7.23279 LUMO: 0.33470 factor:1 | 1 (-1.23172) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.09871 HOMO: -7.17020 LUMO: 0.41361 factor:1 | 1 (-1.22702) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.03749 HOMO: -6.90353 LUMO: -0.90070 factor:1 | 1 (-0.16580) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06182 HOMO: -7.39061 LUMO: 0.17687 factor:1 | 1 (-0.19013) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.56015 HOMO: -7.16748 LUMO: 0.42178 factor:1 | -1 (0.31154) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.71044 HOMO: -7.36884 LUMO: -1.11295 factor:1 | -1 (0.16125) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06837 HOMO: -7.33347 LUMO: 0.33198 factor:1 | 1 (-0.19668) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.00930 HOMO: -7.31986 LUMO: -0.83539 factor:1 | 1 (-0.13761) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58905 HOMO: -7.31170 LUMO: 0.08708 factor:1 | -1 (0.28264) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62431 HOMO: -7.36884 LUMO: 0.38096 factor:1 | -1 (0.24738) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77846 HOMO: -6.99333 LUMO: 1.74153 factor:1 | -1 (0.09323) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.12867 HOMO: -6.94435 LUMO: 1.74969 factor:1 | 1 (-1.25698) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.09098 HOMO: -7.02598 LUMO: 1.43404 factor:1 | 1 (-1.21929) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.49044 HOMO: -6.41100 LUMO: 1.62996 factor:1 | 1 (-1.61875) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.65080 HOMO: -6.57699 LUMO: 1.81228 factor:1 | 1 (-1.77911) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.52835 HOMO: -6.86543 LUMO: 1.49935 factor:1 | 1 (-1.65666) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.36824 HOMO: -6.91169 LUMO: -1.22451 factor:1 | 1 (-1.49654) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.68802 HOMO: -7.09945 LUMO: -1.23812 factor:1 | 1 (-1.81633) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.67687 HOMO: -7.48857 LUMO: 0.10340 factor:1 | 1 (-1.80518) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.73821 HOMO: -7.21918 LUMO: -0.06803 factor:1 | 1 (-0.86652) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.48190 HOMO: -6.34025 LUMO: -0.68845 factor:1 | 1 (-1.61021) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.88447 HOMO: -6.82734 LUMO: -0.77825 factor:1 | 1 (-1.01278) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.04639 HOMO: -6.92258 LUMO: -1.03675 factor:1 | 1 (-0.17470) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05444 HOMO: -6.42461 LUMO: -0.95240 factor:1 | 1 (-0.18275) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58086 HOMO: -6.96067 LUMO: -1.05036 factor:1 | -1 (0.29084) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68521 HOMO: -7.23551 LUMO: 0.12245 factor:1 | -1 (0.18648) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.53095 HOMO: -6.85183 LUMO: 0.16055 factor:1 | -1 (0.34074) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.34662 HOMO: -6.46815 LUMO: -0.89253 factor:1 | -1 (0.52507) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17540 HOMO: -7.23823 LUMO: -0.06259 factor:1 | 1 (-0.30371) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.17830 HOMO: -6.76475 LUMO: -0.99049 factor:1 | 1 (-1.30661) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.32792 HOMO: -7.14843 LUMO: -0.88165 factor:1 | 1 (-0.45623) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.05574 HOMO: -7.15659 LUMO: 0.20681 factor:1 | 1 (-1.18405) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.31724 HOMO: -7.11306 LUMO: 0.14150 factor:1 | 1 (-1.44555) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.46084 HOMO: -6.67223 LUMO: -0.86260 factor:1 | 1 (-0.58915) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.31924 HOMO: -6.92530 LUMO: 0.30749 factor:1 | 1 (-0.44755) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.01220 HOMO: -6.50624 LUMO: -0.70477 factor:1 | 1 (-1.14051) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50452 HOMO: -7.35524 LUMO: 0.75103 factor:1 | 1 (-0.63283) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.66818 HOMO: -7.07768 LUMO: -0.26939 factor:1 | -1 (0.20351) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.72578 HOMO: -7.15932 LUMO: 0.42450 factor:1 | -1 (0.14591) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.63538 HOMO: -7.46136 LUMO: 0.04626 factor:1 | 1 (-0.76369) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.04173 HOMO: -7.05047 LUMO: -1.06669 factor:1 | 1 (-1.17004) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79759 HOMO: -6.66951 LUMO: -0.99322 factor:1 | 1 (-0.92589) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76706 HOMO: -7.01782 LUMO: -1.08846 factor:1 | -1 (0.10463) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59792 HOMO: -7.03959 LUMO: -1.15376 factor:1 | -1 (0.27377) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.70390 HOMO: -6.68856 LUMO: 1.61364 factor:1 | 1 (-0.83221) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.78368 HOMO: -6.53345 LUMO: 1.60275 factor:1 | 1 (-0.91199) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.42952 HOMO: -6.73482 LUMO: 1.86398 factor:1 | 1 (-0.55783) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.76266 HOMO: -6.87632 LUMO: 1.59731 factor:1 | -1 (1.10903) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.66984 HOMO: -6.31848 LUMO: 2.12521 factor:1 | -1 (0.20185) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.37815 HOMO: -6.35114 LUMO: 1.71432 factor:1 | 1 (-0.50646) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.51881 HOMO: -6.34842 LUMO: 1.92929 factor:1 | -1 (0.35288) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.91049 HOMO: -6.14977 LUMO: 1.78235 factor:1 | 1 (-1.03879) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.07384 HOMO: -6.31032 LUMO: 1.51567 factor:1 | 1 (-1.20214) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45810 HOMO: -6.25862 LUMO: 1.75241 factor:1 | -1 (0.41359) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61617 HOMO: -6.49264 LUMO: 1.66806 factor:1 | 1 (-0.74448) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.04017 HOMO: -6.28311 LUMO: 1.60003 factor:1 | -1 (0.83153) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.30123 HOMO: -7.13210 LUMO: -0.04354 factor:1 | -1 (0.57046) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.87318 HOMO: -7.35252 LUMO: 0.03537 factor:1 | 1 (-1.00149) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.45252 HOMO: -6.58243 LUMO: -0.48980 factor:1 | 1 (-0.58083) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.04880 HOMO: -6.90081 LUMO: -0.05442 factor:1 | 1 (-1.17711) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.59189 HOMO: -7.22734 LUMO: 0.17143 factor:1 | 1 (-0.72020) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.77973 HOMO: -7.13210 LUMO: -0.99866 factor:1 | 1 (-0.90804) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17442 HOMO: -7.39878 LUMO: 0.13334 factor:1 | 1 (-0.30273) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57982 HOMO: -7.04503 LUMO: -0.89798 factor:1 | -1 (0.29187) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68630 HOMO: -6.95523 LUMO: -1.07213 factor:1 | -1 (0.18539) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.45831 HOMO: -6.75114 LUMO: -1.28438 factor:1 | 1 (-0.58662) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.28711 HOMO: -6.75114 LUMO: -0.11701 factor:1 | -1 (0.58458) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58747 HOMO: -6.83278 LUMO: -0.01633 factor:1 | -1 (0.28422) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.86653 HOMO: -6.93890 LUMO: -0.88981 factor:1 | -1 (1.00516) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88976 HOMO: -7.07224 LUMO: -1.08573 factor:1 | 1 (-0.01807) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.37310 HOMO: -6.99877 LUMO: -0.95240 factor:1 | -1 (0.49859) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96312 HOMO: -7.09129 LUMO: 0.35375 factor:1 | 1 (-0.09143) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.02123 HOMO: -7.09401 LUMO: 0.04354 factor:1 | -1 (0.85046) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.71464 HOMO: -6.85183 LUMO: -0.68573 factor:1 | -1 (1.15706) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69629 HOMO: -6.83006 LUMO: -0.58777 factor:1 | -1 (0.17540) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.92206 HOMO: -7.40422 LUMO: 0.17687 factor:1 | 1 (-0.05037) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27024 HOMO: -7.15932 LUMO: 0.10340 factor:1 | -1 (0.60145) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.98675 HOMO: -7.03414 LUMO: -0.19592 factor:1 | -1 (0.88494) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69751 HOMO: -6.48447 LUMO: -0.36191 factor:1 | -1 (0.17418) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05039 HOMO: -7.49402 LUMO: 0.11429 factor:1 | 1 (-0.17870) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.62327 HOMO: -7.01237 LUMO: -1.06397 factor:1 | 1 (-0.75158) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88383 HOMO: -6.67223 LUMO: -1.07213 factor:1 | 1 (-0.01214) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.55737 HOMO: -7.38789 LUMO: -1.15376 factor:1 | -1 (0.31432) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.26983 HOMO: -6.42461 LUMO: -1.23812 factor:1 | -1 (0.60186) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59345 HOMO: -7.36884 LUMO: -1.19186 factor:1 | -1 (0.27824) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46572 HOMO: -6.65591 LUMO: 0.07075 factor:1 | -1 (0.40597) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70061 HOMO: -7.39061 LUMO: -0.16871 factor:1 | -1 (0.17108) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81909 HOMO: -6.90353 LUMO: -0.96056 factor:1 | -1 (0.05260) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.02703 HOMO: -7.42054 LUMO: 0.19048 factor:1 | 1 (-1.15534) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.29177 HOMO: -7.40150 LUMO: 0.35647 factor:1 | 1 (-1.42008) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61236 HOMO: -6.56067 LUMO: -0.96056 factor:1 | 1 (-0.74067) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36473 HOMO: -6.89809 LUMO: -0.81090 factor:1 | 1 (-0.49304) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77212 HOMO: -6.91986 LUMO: -0.84900 factor:1 | -1 (0.09957) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.24160 HOMO: -6.61509 LUMO: -0.62042 factor:1 | 1 (-0.36991) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.66635 HOMO: -6.58243 LUMO: -0.65579 factor:1 | -1 (0.20534) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27451 HOMO: -6.52257 LUMO: -0.92519 factor:1 | -1 (0.59718) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05463 HOMO: -6.69128 LUMO: 1.49118 factor:1 | 1 (-0.18294) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58706 HOMO: -7.02870 LUMO: 1.67894 factor:1 | -1 (0.28463) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81041 HOMO: -6.88720 LUMO: 1.68711 factor:1 | -1 (0.06128) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.75579 HOMO: -5.89943 LUMO: 1.03675 factor:1 | 1 (-0.88410) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.23822 HOMO: -6.40556 LUMO: 1.14560 factor:1 | 1 (-1.36653) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.67630 HOMO: -6.51168 LUMO: 1.48030 factor:1 | 1 (-0.80461) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.47872 HOMO: -6.64502 LUMO: 1.91568 factor:1 | 1 (-0.60703) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.69481 HOMO: -6.47903 LUMO: 1.91296 factor:1 | 1 (-0.82312) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27119 HOMO: -6.34297 LUMO: 1.91840 factor:1 | -1 (0.60050) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.04114 HOMO: -6.89809 LUMO: 1.82861 factor:1 | -1 (0.83055) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.31160 HOMO: -6.10079 LUMO: 1.62996 factor:1 | -1 (0.56009) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.42537 HOMO: -7.16476 LUMO: -0.92247 factor:1 | -1 (0.44632) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.24509 HOMO: -7.10489 LUMO: -0.95784 factor:1 | -1 (0.62660) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.26678 HOMO: -6.76475 LUMO: -0.99866 factor:1 | -1 (0.60491) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.22085 HOMO: -6.81373 LUMO: -1.05036 factor:1 | -1 (0.65084) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79440 HOMO: -6.90081 LUMO: -1.03947 factor:1 | 1 (-0.92271) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80168 HOMO: -7.06952 LUMO: -0.91702 factor:1 | -1 (0.07001) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.37692 HOMO: -6.73482 LUMO: -0.94151 factor:1 | 1 (-1.50523) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.64773 HOMO: -6.99605 LUMO: -1.04764 factor:1 | 1 (-0.77604) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.39358 HOMO: -7.03686 LUMO: -0.93335 factor:1 | 1 (-0.52189) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.70537 HOMO: -6.81101 LUMO: -0.95240 factor:1 | 1 (-0.83368) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.38289 HOMO: -6.83822 LUMO: -0.65307 factor:1 | -1 (0.48880) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.43651 HOMO: -7.05319 LUMO: -0.81634 factor:1 | -1 (1.43518) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.10047 HOMO: -7.57565 LUMO: 0.19048 factor:1 | -1 (0.77123) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.40044 HOMO: -6.56067 LUMO: -0.50613 factor:1 | 1 (-0.52874) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.56842 HOMO: -6.74298 LUMO: -0.70477 factor:1 | -1 (0.30327) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.37214 HOMO: -7.02054 LUMO: 0.03537 factor:1 | -1 (0.49955) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.12261 HOMO: -7.33347 LUMO: -0.17960 factor:1 | 1 (-0.25092) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.18441 HOMO: -6.98244 LUMO: -0.88165 factor:1 | -1 (0.68728) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.38574 HOMO: -7.14843 LUMO: -1.19730 factor:1 | 1 (-0.51405) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.49870 HOMO: -7.17564 LUMO: -1.21907 factor:1 | -1 (0.37299) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.32858 HOMO: -6.74026 LUMO: -0.86532 factor:1 | -1 (0.54311) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11670 HOMO: -6.82462 LUMO: -1.24084 factor:1 | 1 (-0.24501) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.55808 HOMO: -6.78924 LUMO: -0.70477 factor:1 | -1 (0.31361) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.15156 HOMO: -7.41238 LUMO: 0.05987 factor:1 | 1 (-0.27987) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.25738 HOMO: -6.75931 LUMO: 0.02721 factor:1 | -1 (2.61431) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.97332 HOMO: -6.28583 LUMO: -0.93063 factor:1 | -1 (1.89838) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.61589 HOMO: -6.69128 LUMO: -0.83539 factor:1 | -1 (2.25580) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.92113 HOMO: -7.22190 LUMO: 0.01361 factor:1 | 1 (-0.04944) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45740 HOMO: -6.95251 LUMO: -1.09934 factor:1 | -1 (0.41429) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.13640 HOMO: -6.75387 LUMO: -0.90614 factor:1 | 1 (-0.26471) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.99145 HOMO: -7.48585 LUMO: 0.05987 factor:1 | 1 (-0.11976) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.61928 HOMO: -6.92802 LUMO: -0.66940 factor:1 | -1 (0.25241) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.36964 HOMO: -7.29537 LUMO: -0.14150 factor:1 | -1 (0.50205) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.02307 HOMO: -6.57155 LUMO: -0.86804 factor:1 | 1 (-0.15138) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.13224 HOMO: -6.87632 LUMO: -0.77825 factor:1 | 1 (-0.26055) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.04271 HOMO: -6.45998 LUMO: -0.31565 factor:1 | 1 (-0.17102) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.10205 HOMO: -7.51306 LUMO: 0.05714 factor:1 | -1 (1.76964) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76168 HOMO: -6.86271 LUMO: -0.00816 factor:1 | -1 (0.11002) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.64851 HOMO: -6.43277 LUMO: -1.07485 factor:1 | -1 (1.22318) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.11824 HOMO: -6.78108 LUMO: -0.81362 factor:1 | 1 (-1.24655) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23907 HOMO: -6.88448 LUMO: 1.21907 factor:1 | 1 (-0.36738) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.98208 HOMO: -6.97700 LUMO: 1.44765 factor:1 | 1 (-1.11039) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.07852 HOMO: -6.89537 LUMO: 2.12249 factor:1 | 1 (-0.20683) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.09800 HOMO: -6.28311 LUMO: 1.45037 factor:1 | 1 (-1.22631) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.22089 HOMO: -6.55522 LUMO: 1.39867 factor:1 | 1 (-0.34920) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.69873 HOMO: -6.46815 LUMO: 1.50207 factor:1 | 1 (-0.82704) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96549 HOMO: -6.43549 LUMO: 2.17419 factor:1 | 1 (-0.09380) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.20243 HOMO: -6.99333 LUMO: 1.87214 factor:1 | -1 (0.66926) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.80620 HOMO: -6.65591 LUMO: 1.37962 factor:1 | -1 (1.06549) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58086 HOMO: -6.82734 LUMO: 1.55649 factor:1 | -1 (0.29084) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.93403 HOMO: -6.71849 LUMO: 1.36057 factor:1 | 1 (-0.06234) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.57238 HOMO: -6.79468 LUMO: 1.82044 factor:1 | 1 (-0.70069) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.82689 HOMO: -6.61237 LUMO: 1.15104 factor:1 | 1 (-0.95520) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14043 HOMO: -6.62053 LUMO: 2.33474 factor:1 | 1 (-0.26874) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80535 HOMO: -6.55794 LUMO: 1.65717 factor:1 | -1 (0.06634) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.70413 HOMO: -6.85999 LUMO: 2.03813 factor:1 | -1 (1.16756) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.90834 HOMO: -6.45726 LUMO: 1.28438 factor:1 | 1 (-0.03665) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.22364 HOMO: -6.23685 LUMO: 1.93201 factor:1 | 1 (-0.35195) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.76828 HOMO: -7.06680 LUMO: 1.86942 factor:1 | -1 (2.10341) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.34349 HOMO: -6.89537 LUMO: 2.17147 factor:1 | -1 (0.52820) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.94209 HOMO: -6.80013 LUMO: 1.78779 factor:1 | 1 (-0.07040) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.09998 HOMO: -6.45726 LUMO: 1.58370 factor:1 | -1 (0.77171) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.76236 HOMO: -6.52529 LUMO: 1.71976 factor:1 | -1 (1.10933) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.63512 HOMO: -7.22462 LUMO: -1.18642 factor:1 | -1 (0.23658) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69259 HOMO: -7.18381 LUMO: -0.78641 factor:1 | -1 (0.17911) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58951 HOMO: -6.93346 LUMO: 1.65717 factor:1 | -1 (0.28218) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.49040 HOMO: -6.41644 LUMO: 1.78235 factor:1 | -1 (0.38129) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.90218 HOMO: -6.59876 LUMO: 1.83677 factor:1 | -1 (0.96951) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85215 HOMO: -6.35658 LUMO: 1.59731 factor:1 | -1 (0.01954) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.20697 HOMO: -6.60692 LUMO: 1.66534 factor:1 | -1 (0.66472) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.07647 HOMO: -6.83006 LUMO: 2.11705 factor:1 | -1 (0.79523) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62143 HOMO: -6.89264 LUMO: 1.30070 factor:1 | -1 (0.25026) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.74631 HOMO: -6.90081 LUMO: 2.05174 factor:1 | -1 (1.12538) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01597 HOMO: -6.74842 LUMO: 1.96194 factor:1 | 1 (-0.14427) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.95011 HOMO: -6.58516 LUMO: 1.30887 factor:1 | 1 (-0.07842) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76018 HOMO: -7.00965 LUMO: 2.08167 factor:1 | -1 (0.11151) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.89576 HOMO: -6.86815 LUMO: 2.29664 factor:1 | -1 (1.97593) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60935 HOMO: -6.39740 LUMO: 2.02725 factor:1 | -1 (0.26234) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96617 HOMO: -5.95929 LUMO: 1.62724 factor:1 | 1 (-0.09448) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.09541 HOMO: -6.71849 LUMO: 1.34696 factor:1 | -1 (1.77628) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.08568 HOMO: -7.26816 LUMO: 1.74153 factor:1 | 1 (-0.21399) | 1 | 1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.67724 HOMO: -6.90897 LUMO: 1.71432 factor:1 | -1 (0.19445) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.58516 HOMO: -6.70489 LUMO: 1.91568 factor:1 | -1 (1.28653) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.33628 HOMO: -6.83278 LUMO: 1.61908 factor:1 | -1 (0.53541) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.51972 HOMO: -7.17292 LUMO: 1.95378 factor:1 | -1 (1.35197) | 1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.53351 HOMO: -6.53345 LUMO: 1.74153 factor:1 | -1 (0.33818) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45198 HOMO: -6.53073 LUMO: 1.51023 factor:1 | -1 (0.41971) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.37565 HOMO: -6.93346 LUMO: 2.22861 factor:1 | -1 (0.49604) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.90829 HOMO: -6.47903 LUMO: 2.05446 factor:1 | 1 (-0.03660) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.67283 HOMO: -6.88992 LUMO: 1.57010 factor:1 | -1 (0.19886) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96062 HOMO: -6.07358 LUMO: 1.95922 factor:1 | 1 (-0.08893) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.75634 HOMO: -6.75114 LUMO: 2.18780 factor:1 | -1 (0.11535) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.98609 HOMO: -6.96339 LUMO: 1.70071 factor:1 | 1 (-0.11440) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.78306 HOMO: -7.14843 LUMO: 1.82588 factor:1 | -1 (0.08863) | 1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.74805 HOMO: -6.96339 LUMO: 2.29392 factor:1 | -1 (1.12364) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.53781 HOMO: -6.81645 LUMO: 2.39732 factor:1 | -1 (0.33388) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.55896 HOMO: -6.48447 LUMO: 1.24084 factor:1 | -1 (1.31273) | -1 | -1 |
| G: -6695.50600 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.21162 HOMO: -7.14843 LUMO: 2.01092 factor:1 | -1 (0.66007) | 1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.28574 HOMO: -7.20013 LUMO: -0.34286 factor:1 | -1 (2.58595) | 1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.93187 HOMO: -6.97700 LUMO: -0.15238 factor:1 | -1 (1.93982) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.64926 HOMO: -7.07768 LUMO: -0.26123 factor:1 | -1 (2.22244) | 1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77901 HOMO: -6.99333 LUMO: -0.41361 factor:1 | -1 (0.09268) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57408 HOMO: -6.84638 LUMO: -0.40273 factor:1 | -1 (0.29761) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.82932 HOMO: -6.83822 LUMO: -0.26939 factor:1 | -1 (0.04237) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.92955 HOMO: -6.75931 LUMO: -0.93879 factor:1 | -1 (0.94214) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.78731 HOMO: -6.79468 LUMO: -0.39729 factor:1 | -1 (0.08438) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69109 HOMO: -6.93890 LUMO: 0.43266 factor:1 | -1 (0.18060) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.56336 HOMO: -7.08040 LUMO: -0.85716 factor:1 | -1 (0.30833) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.97395 HOMO: -6.70216 LUMO: -1.41499 factor:1 | 1 (-0.10226) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89267 HOMO: -6.63686 LUMO: -0.52790 factor:1 | 1 (-0.02098) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.95294 HOMO: -6.75114 LUMO: -0.13334 factor:1 | 1 (-0.08125) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.19138 HOMO: -6.94435 LUMO: -0.24490 factor:1 | -1 (0.68031) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.25718 HOMO: -6.74298 LUMO: -0.84627 factor:1 | -1 (1.61451) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.36872 HOMO: -7.15932 LUMO: 0.22041 factor:1 | -1 (0.50298) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.50075 HOMO: -6.90081 LUMO: -1.16737 factor:1 | -1 (1.37094) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46605 HOMO: -7.04775 LUMO: -0.84355 factor:1 | -1 (0.40564) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.27861 HOMO: -7.17020 LUMO: -1.31159 factor:1 | 1 (-0.40692) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.33692 HOMO: -7.14571 LUMO: -0.46259 factor:1 | 1 (-0.46523) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62004 HOMO: -7.45048 LUMO: -0.91158 factor:1 | -1 (0.25165) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61992 HOMO: -6.87360 LUMO: -0.82995 factor:1 | 1 (-0.74823) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.92252 HOMO: -7.43415 LUMO: -0.65307 factor:1 | 1 (-0.05083) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.02664 HOMO: -7.47225 LUMO: -0.77280 factor:1 | -1 (0.84505) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.61884 HOMO: -6.86271 LUMO: -0.83811 factor:1 | -1 (0.25285) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.97738 HOMO: -7.53483 LUMO: -0.66124 factor:1 | 1 (-0.10569) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.94568 HOMO: -7.45864 LUMO: -1.08301 factor:1 | 1 (-0.07399) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.38009 HOMO: -7.24639 LUMO: -1.19186 factor:1 | -1 (0.49160) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.65612 HOMO: -7.54844 LUMO: -0.96873 factor:1 | -1 (0.21557) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.54224 HOMO: -7.12666 LUMO: -0.01633 factor:1 | -1 (0.32945) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.95695 HOMO: -6.77291 LUMO: -0.70477 factor:1 | -1 (0.91474) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80823 HOMO: -6.76475 LUMO: -1.15921 factor:1 | -1 (0.06346) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.24216 HOMO: -5.37697 LUMO: -0.56600 factor:1 | -1 (0.62954) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.97998 HOMO: -6.62053 LUMO: -1.75513 factor:1 | 1 (-1.10829) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17336 HOMO: -6.60420 LUMO: -1.74697 factor:1 | 1 (-0.30167) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.98513 HOMO: -6.84366 LUMO: -0.94968 factor:1 | 1 (-1.11344) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01308 HOMO: -6.96884 LUMO: -2.11977 factor:1 | 1 (-0.14139) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23692 HOMO: -6.80829 LUMO: 0.56055 factor:1 | 1 (-0.36523) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.04978 HOMO: -7.02326 LUMO: 0.11429 factor:1 | 1 (-1.17809) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.55709 HOMO: -7.40966 LUMO: 0.18232 factor:1 | 1 (-0.68540) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91942 HOMO: -6.34570 LUMO: 0.41089 factor:1 | 1 (-0.04773) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.10855 HOMO: -6.78924 LUMO: 0.49525 factor:1 | -1 (0.76314) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.02729 HOMO: -6.87632 LUMO: 0.44082 factor:1 | 1 (-0.15559) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.94466 HOMO: -6.69944 LUMO: 1.20546 factor:1 | 1 (-1.07297) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.56419 HOMO: -6.83006 LUMO: 1.28982 factor:1 | 1 (-0.69250) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.97931 HOMO: -7.78246 LUMO: 0.20681 factor:1 | 1 (-0.10762) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.94088 HOMO: -6.55794 LUMO: -1.65173 factor:1 | 1 (-1.06919) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.57943 HOMO: -6.77564 LUMO: -1.14560 factor:1 | 1 (-0.70774) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.94750 HOMO: -7.46680 LUMO: -1.18097 factor:1 | 1 (-0.07581) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.60166 HOMO: -6.88176 LUMO: -1.24900 factor:1 | 1 (-0.72997) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.09284 HOMO: -7.28177 LUMO: -0.42178 factor:1 | 1 (-0.22115) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.95866 HOMO: -7.71715 LUMO: 0.19592 factor:1 | 1 (-0.08697) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.24833 HOMO: -7.02326 LUMO: -1.40683 factor:1 | -1 (0.62336) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87479 HOMO: -7.27088 LUMO: -1.07485 factor:1 | 1 (-0.00310) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.67055 HOMO: -7.17020 LUMO: -0.49525 factor:1 | -1 (1.20114) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.05802 HOMO: -7.15932 LUMO: 0.02721 factor:1 | -1 (0.81367) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.87593 HOMO: -7.00693 LUMO: -0.83267 factor:1 | -1 (1.99576) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01156 HOMO: -6.86543 LUMO: -0.10340 factor:1 | 1 (-0.13987) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.65708 HOMO: -7.11850 LUMO: -0.08980 factor:1 | -1 (1.21461) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.84233 HOMO: -6.87087 LUMO: -0.88981 factor:1 | -1 (0.02936) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.79991 HOMO: -7.08857 LUMO: -1.27077 factor:1 | -1 (0.07178) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91145 HOMO: -6.79468 LUMO: -0.81906 factor:1 | 1 (-0.03976) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.07205 HOMO: -6.86815 LUMO: -0.89798 factor:1 | 1 (-0.20036) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.12973 HOMO: -6.78652 LUMO: -2.00548 factor:1 | -1 (1.74196) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.81083 HOMO: -6.75114 LUMO: -0.08436 factor:1 | -1 (1.06086) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68695 HOMO: -6.55794 LUMO: 0.52790 factor:1 | -1 (0.18474) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.43514 HOMO: -7.17836 LUMO: 0.28300 factor:1 | -1 (0.43655) | 1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68140 HOMO: -7.35796 LUMO: -0.77552 factor:1 | -1 (0.19029) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.29108 HOMO: -7.23551 LUMO: -1.17553 factor:1 | -1 (0.58061) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.90838 HOMO: -7.07496 LUMO: -1.14288 factor:1 | -1 (0.96331) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.66348 HOMO: -6.70489 LUMO: -0.83539 factor:1 | -1 (1.20821) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.84064 HOMO: -6.59604 LUMO: -0.89798 factor:1 | -1 (0.03105) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80921 HOMO: -6.94162 LUMO: -1.22451 factor:1 | -1 (0.06248) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.10993 HOMO: -6.68040 LUMO: 0.22041 factor:1 | 1 (-0.23824) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.86388 HOMO: -6.88176 LUMO: 0.11157 factor:1 | -1 (0.00781) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.14634 HOMO: -6.91713 LUMO: 1.27621 factor:1 | -1 (0.72535) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45576 HOMO: -6.77836 LUMO: 1.01226 factor:1 | -1 (0.41593) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.52639 HOMO: -7.14571 LUMO: 1.48574 factor:1 | -1 (1.34530) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.61840 HOMO: -6.96884 LUMO: 1.48574 factor:1 | -1 (2.25329) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87890 HOMO: -7.24367 LUMO: 1.28438 factor:1 | 1 (-0.00721) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.86932 HOMO: -7.10489 LUMO: 1.29526 factor:1 | -1 (0.00237) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64967 HOMO: -7.07224 LUMO: 1.29254 factor:1 | -1 (0.22202) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59413 HOMO: -7.12938 LUMO: 0.49253 factor:1 | -1 (0.27756) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60826 HOMO: -7.33619 LUMO: 1.45581 factor:1 | -1 (0.26343) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.61672 HOMO: -6.87904 LUMO: -0.14422 factor:1 | -1 (0.25497) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.78384 HOMO: -6.81917 LUMO: 0.50341 factor:1 | 1 (-0.91215) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.33698 HOMO: -7.27905 LUMO: 0.13606 factor:1 | 1 (-0.46529) | 1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62967 HOMO: -6.87904 LUMO: -0.09796 factor:1 | -1 (0.24202) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20190 HOMO: -7.33891 LUMO: 0.03810 factor:1 | 1 (-0.33021) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36838 HOMO: -6.98516 LUMO: 0.98233 factor:1 | 1 (-0.49669) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.57002 HOMO: -6.94162 LUMO: 0.86804 factor:1 | 1 (-0.69833) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.86293 HOMO: -7.37701 LUMO: 0.05442 factor:1 | -1 (0.00876) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70861 HOMO: -7.04775 LUMO: 0.43266 factor:1 | -1 (0.16308) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30277 HOMO: -7.47497 LUMO: 0.31837 factor:1 | 1 (-0.43108) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50645 HOMO: -6.62053 LUMO: 0.13061 factor:1 | 1 (-0.63476) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45898 HOMO: -6.44366 LUMO: -0.04354 factor:1 | -1 (0.41272) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46330 HOMO: -6.40284 LUMO: 0.68301 factor:1 | -1 (0.40839) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.35614 HOMO: -6.73754 LUMO: 0.36735 factor:1 | 1 (-0.48444) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.72251 HOMO: -6.85455 LUMO: 0.23946 factor:1 | 1 (-0.85082) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52050 HOMO: -6.93346 LUMO: 0.24762 factor:1 | -1 (0.35119) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68597 HOMO: -6.85455 LUMO: 0.17687 factor:1 | -1 (0.18572) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11665 HOMO: -6.62325 LUMO: 0.69933 factor:1 | 1 (-0.24496) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.71686 HOMO: -6.43005 LUMO: 0.50069 factor:1 | -1 (0.15483) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70184 HOMO: -6.56883 LUMO: 0.22858 factor:1 | -1 (0.16985) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.84173 HOMO: -6.78380 LUMO: 0.54967 factor:1 | -1 (0.02996) | -1 | -1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.77983 HOMO: -7.35524 LUMO: 0.00272 factor:1 | -1 (1.09186) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.47857 HOMO: -7.27360 LUMO: 0.08436 factor:1 | -1 (0.39312) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62608 HOMO: -7.44504 LUMO: -0.96056 factor:1 | -1 (0.24561) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.39519 HOMO: -7.27360 LUMO: 0.29933 factor:1 | -1 (0.47650) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77719 HOMO: -7.09129 LUMO: 0.41089 factor:1 | -1 (0.09451) | 1 | 1 |
| G: -6695.50600 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.75977 HOMO: -6.93618 LUMO: 0.36463 factor:1 | -1 (0.11192) | -1 | -1 |
| G: -6695.50600 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.40375 HOMO: -7.65728 LUMO: 0.20136 factor:1 | -1 (2.46794) | 1 | 1 |
| G: -6695.50600 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89444 HOMO: -6.90353 LUMO: -0.92791 factor:1 | 1 (-0.02275) | -1 | -1 |
| G: -6695.50600 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76758 HOMO: -6.82462 LUMO: -1.18370 factor:1 | -1 (0.10411) | -1 | -1 |
| G: -6695.50600 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.66015 HOMO: -7.09129 LUMO: -0.13334 factor:1 | -1 (0.21154) | 1 | 1 |
| G: -6695.50600 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45710 HOMO: -7.40966 LUMO: -1.06941 factor:1 | -1 (0.41459) | 1 | 1 |
| G: -6695.50600 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.61768 HOMO: -7.24367 LUMO: -1.00954 factor:1 | -1 (1.25401) | 1 | 1 |
| G: -6695.50600 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.86847 HOMO: -7.51851 LUMO: 0.09796 factor:1 | 1 (-0.99678) | 1 | 1 |
| G: -6695.50600 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91063 HOMO: -7.48857 LUMO: -0.07619 factor:1 | 1 (-0.03894) | 1 | 1 |
| G: -6695.50600 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.12857 HOMO: -6.53345 LUMO: 1.09390 factor:1 | 1 (-0.25688) | -1 | -1 |
| G: -6695.50600 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46262 HOMO: -7.21918 LUMO: 0.08436 factor:1 | -1 (0.40907) | 1 | 1 |
| G: -6695.50600 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77700 HOMO: -7.38789 LUMO: 1.02587 factor:1 | -1 (0.09470) | 1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.92074 HOMO: -6.83550 LUMO: -0.67484 factor:1 | 1 (-1.04905) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.90108 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-0.02939) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.85448 HOMO: -6.79740 LUMO: 1.91296 factor:1 | 1 (-0.98279) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17564 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-0.30395) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50864 HOMO: -6.62597 LUMO: -0.44082 factor:1 | -1 (0.36305) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.28571 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-0.41402) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80864 HOMO: -6.51168 LUMO: -0.23130 factor:1 | -1 (0.06305) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62970 HOMO: -7.14027 LUMO: 0.49797 factor:1 | -1 (0.24199) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.36270 HOMO: -7.55660 LUMO: 0.24762 factor:1 | -1 (0.50899) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.38619 HOMO: -6.88992 LUMO: -0.64763 factor:1 | -1 (0.48551) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89670 HOMO: -6.72665 LUMO: -0.45987 factor:1 | 1 (-0.02501) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.36447 HOMO: -6.72121 LUMO: -0.58232 factor:1 | -1 (0.50722) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.15551 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-0.28381) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.43410 HOMO: -6.57155 LUMO: -0.53606 factor:1 | -1 (0.43759) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.75460 HOMO: -6.50896 LUMO: -0.43810 factor:1 | -1 (0.11709) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.09850 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-0.22681) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.34879 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-0.47710) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52140 HOMO: -6.82462 LUMO: -0.67484 factor:1 | -1 (0.35029) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.36531 HOMO: -6.79740 LUMO: -0.55511 factor:1 | -1 (0.50638) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.42842 HOMO: -6.79740 LUMO: -0.67756 factor:1 | -1 (0.44327) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.52971 HOMO: -6.75114 LUMO: -0.55239 factor:1 | -1 (1.34198) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36887 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-0.49718) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64121 HOMO: -6.48992 LUMO: -0.25034 factor:1 | -1 (0.23048) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20963 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-0.33794) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27998 HOMO: -7.22462 LUMO: 0.52518 factor:1 | -1 (0.59171) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91847 HOMO: -6.59332 LUMO: -0.27211 factor:1 | 1 (-0.04678) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.77797 HOMO: -6.57427 LUMO: -0.16871 factor:1 | 1 (-0.90628) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.40737 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-1.53567) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.15749 HOMO: -6.72121 LUMO: 2.00004 factor:1 | 1 (-0.28580) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.62558 HOMO: -6.61509 LUMO: 1.55921 factor:1 | 1 (-0.75389) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.41448 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-0.54279) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.48097 HOMO: -6.66135 LUMO: 2.02181 factor:1 | 1 (-1.60928) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.84379 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-0.97210) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.48689 HOMO: -6.66679 LUMO: 1.98371 factor:1 | 1 (-0.61520) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.99975 HOMO: -6.67495 LUMO: 2.04085 factor:1 | 1 (-0.12806) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46333 HOMO: -6.89809 LUMO: 1.95106 factor:1 | -1 (0.40836) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.91280 HOMO: -6.50352 LUMO: 1.88847 factor:1 | 1 (-1.04111) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11510 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-0.24341) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.63297 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-1.76128) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.93868 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-1.06699) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.52000 HOMO: -6.65591 LUMO: 2.20684 factor:1 | 1 (-0.64831) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.72120 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-0.84951) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.18657 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-1.31488) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.55840 HOMO: -6.53617 LUMO: 1.75241 factor:1 | 1 (-0.68671) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.79132 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-1.91963) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.84552 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-1.97383) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.38163 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-0.50994) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.66313 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-0.79144) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.94981 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-1.07812) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.21796 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-0.34626) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.03471 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-1.16301) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36177 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-0.49008) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.97749 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-0.10580) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.08554 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-1.21385) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.09860 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-1.22691) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.44950 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-0.57781) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01771 HOMO: -6.90897 LUMO: 1.91296 factor:1 | 1 (-0.14602) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.48778 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-1.61608) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.41771 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-0.54602) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.12744 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-1.25575) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.29902 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-0.42733) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.32243 HOMO: -7.04231 LUMO: 1.79323 factor:1 | -1 (0.54926) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36653 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-0.49484) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.23562 HOMO: -6.40556 LUMO: 1.45581 factor:1 | -1 (0.63607) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30226 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-0.43057) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68350 HOMO: -6.84911 LUMO: 1.89935 factor:1 | -1 (0.18819) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.73081 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-0.85912) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64360 HOMO: -6.51168 LUMO: 2.10072 factor:1 | -1 (0.22809) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.55361 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-0.68192) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.29576 HOMO: -6.84094 LUMO: 1.63268 factor:1 | -1 (0.57593) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57313 HOMO: -6.75387 LUMO: 1.72248 factor:1 | -1 (0.29856) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20402 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-0.33233) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27168 HOMO: -6.84094 LUMO: 2.02997 factor:1 | -1 (0.60001) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.41332 HOMO: -6.80557 LUMO: 2.02725 factor:1 | -1 (0.45838) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.96192 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-1.09022) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61946 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-0.74777) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50501 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-0.63332) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.71266 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-0.84097) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20000 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-0.32831) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.15173 HOMO: -6.60692 LUMO: -0.22313 factor:1 | -1 (0.71996) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.38362 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-0.51193) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.41356 HOMO: -6.60420 LUMO: -0.28028 factor:1 | -1 (0.45813) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17902 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-0.30733) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.55212 HOMO: -6.65591 LUMO: -0.25579 factor:1 | -1 (0.31957) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64679 HOMO: -6.69128 LUMO: 1.70888 factor:1 | -1 (0.22490) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.97625 HOMO: -6.50080 LUMO: 1.87759 factor:1 | -1 (0.89545) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.78108 HOMO: -6.85727 LUMO: 1.99187 factor:1 | -1 (0.09061) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.83139 HOMO: -6.58788 LUMO: 1.79051 factor:1 | -1 (0.04030) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.18915 HOMO: -6.64230 LUMO: 2.16058 factor:1 | -1 (0.68254) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68897 HOMO: -6.58788 LUMO: 2.10616 factor:1 | -1 (0.18272) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.48445 HOMO: -7.01782 LUMO: 2.13609 factor:1 | -1 (0.38725) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.82630 HOMO: -6.31304 LUMO: 2.31841 factor:1 | -1 (0.04539) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85049 HOMO: -6.94979 LUMO: 2.07895 factor:1 | -1 (0.02120) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60619 HOMO: -6.88992 LUMO: 2.28031 factor:1 | -1 (0.26550) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.96493 HOMO: -6.66407 LUMO: 2.07623 factor:1 | -1 (0.90677) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64513 HOMO: -6.52529 LUMO: 1.70071 factor:1 | -1 (0.22656) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91517 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-0.04348) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77659 HOMO: -6.55250 LUMO: 1.95378 factor:1 | -1 (0.09510) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.22588 HOMO: -6.24773 LUMO: 1.77962 factor:1 | -1 (0.64581) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76018 HOMO: -6.31304 LUMO: 2.18507 factor:1 | -1 (0.11151) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69691 HOMO: -6.18243 LUMO: 2.01636 factor:1 | -1 (0.17478) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50779 HOMO: -6.99877 LUMO: 2.14970 factor:1 | -1 (0.36390) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.78617 HOMO: -6.72665 LUMO: 2.07079 factor:1 | -1 (0.08553) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85038 HOMO: -6.36202 LUMO: 2.17419 factor:1 | -1 (0.02131) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.10897 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-1.23727) | 1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23409 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-0.36240) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.62047 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-0.74878) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.74325 HOMO: -6.58788 LUMO: 1.83133 factor:1 | -1 (0.12844) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.66594 HOMO: -7.08584 LUMO: 1.91568 factor:1 | 1 (-0.79425) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57038 HOMO: -6.56883 LUMO: 1.81228 factor:1 | -1 (0.30131) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.90790 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-1.03621) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01553 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-0.14384) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.80085 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-0.92916) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80086 HOMO: -6.44094 LUMO: 1.74425 factor:1 | -1 (0.07083) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50333 HOMO: -6.51985 LUMO: 1.84221 factor:1 | -1 (0.36836) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.71781 HOMO: -6.63414 LUMO: -0.24762 factor:1 | -1 (0.15388) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.78820 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-0.91651) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.29681 HOMO: -7.19741 LUMO: 0.58232 factor:1 | 1 (-0.42512) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50899 HOMO: -6.77019 LUMO: -0.56872 factor:1 | -1 (0.36270) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.03004 HOMO: -7.46136 LUMO: 0.28844 factor:1 | -1 (0.84165) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59835 HOMO: -6.60420 LUMO: -0.54151 factor:1 | -1 (0.27334) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.52210 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-0.65041) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.37761 HOMO: -6.81645 LUMO: -0.57144 factor:1 | -1 (0.49408) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.96747 HOMO: -7.48041 LUMO: 0.28572 factor:1 | 1 (-1.09578) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.56051 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-1.68882) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.41821 HOMO: -6.66135 LUMO: -0.41906 factor:1 | -1 (0.45348) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.71622 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-0.84453) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.48064 HOMO: -7.07496 LUMO: -0.63403 factor:1 | -1 (1.39105) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.72281 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-0.85112) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.93552 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-1.06383) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64282 HOMO: -6.50896 LUMO: -0.25034 factor:1 | -1 (0.22887) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60178 HOMO: -7.17564 LUMO: -0.68573 factor:1 | -1 (0.26991) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62126 HOMO: -6.53617 LUMO: -0.30749 factor:1 | -1 (0.25043) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.51776 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-1.64607) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61864 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-0.74695) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.21066 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-0.33897) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.67475 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-0.80306) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.24073 HOMO: -6.62325 LUMO: 2.02725 factor:1 | 1 (-0.36904) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.85606 HOMO: -6.63414 LUMO: 1.91296 factor:1 | 1 (-0.98437) | 1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.44547 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-0.57378) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.64594 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-0.77425) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.26122 HOMO: -6.61237 LUMO: 2.11432 factor:1 | 1 (-0.38953) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.43488 HOMO: -6.62053 LUMO: 2.09256 factor:1 | 1 (-0.56319) | 1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45326 HOMO: -6.78652 LUMO: 2.13609 factor:1 | -1 (0.41843) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27641 HOMO: -6.94707 LUMO: 1.81772 factor:1 | -1 (0.59528) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70116 HOMO: -6.85183 LUMO: 2.12793 factor:1 | -1 (0.17053) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59963 HOMO: -6.81101 LUMO: 1.83949 factor:1 | -1 (0.27206) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59068 HOMO: -6.98788 LUMO: 2.16058 factor:1 | -1 (0.28101) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.92835 HOMO: -6.62869 LUMO: 2.00820 factor:1 | -1 (0.94334) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.65019 HOMO: -6.34025 LUMO: 2.25855 factor:1 | -1 (0.22150) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89858 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-0.02688) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.44415 HOMO: -6.89264 LUMO: 2.27487 factor:1 | -1 (0.42755) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.33788 HOMO: -6.53073 LUMO: 2.20684 factor:1 | 1 (-0.46619) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.51021 HOMO: -6.83278 LUMO: 1.53744 factor:1 | -1 (0.36148) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.22642 HOMO: -6.41917 LUMO: 1.82316 factor:1 | 1 (-0.35473) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.72404 HOMO: -6.56339 LUMO: 1.63813 factor:1 | -1 (0.14765) | -1 | -1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50015 HOMO: -6.88992 LUMO: 1.65173 factor:1 | -1 (0.37154) | 1 | 1 |
| G: -6695.50600 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.26107 HOMO: -6.63141 LUMO: 1.92112 factor:1 | -1 (0.61062) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.63887 HOMO: -6.83822 LUMO: 1.88847 factor:1 | -1 (0.24534) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.02017 HOMO: -6.84638 LUMO: 1.90480 factor:1 | -1 (1.86403) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.96118 HOMO: -6.82462 LUMO: 1.70888 factor:1 | -1 (1.92303) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.84865 HOMO: -6.82734 LUMO: 2.12521 factor:1 | -1 (1.03556) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.03949 HOMO: -6.94435 LUMO: 1.87214 factor:1 | -1 (0.84472) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60491 HOMO: -6.98516 LUMO: 2.51433 factor:1 | -1 (0.27930) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.94545 HOMO: -6.74026 LUMO: 2.15514 factor:1 | -1 (1.93876) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.22447 HOMO: -6.93618 LUMO: 2.54426 factor:1 | -1 (0.65974) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.35449 HOMO: -6.28583 LUMO: 2.53610 factor:1 | -1 (1.52972) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.47621 HOMO: -6.56883 LUMO: 1.94834 factor:1 | -1 (1.40800) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.99465 HOMO: -7.08584 LUMO: 1.99187 factor:1 | -1 (1.88956) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.57031 HOMO: -6.19059 LUMO: 1.99732 factor:1 | -1 (1.31390) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.71790 HOMO: -6.78108 LUMO: 2.03813 factor:1 | -1 (1.16631) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.33816 HOMO: -6.82189 LUMO: 1.77418 factor:1 | -1 (0.54605) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.89367 HOMO: -6.45454 LUMO: 1.78779 factor:1 | -1 (1.99054) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.38072 HOMO: -6.84366 LUMO: 1.77690 factor:1 | -1 (1.50348) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.69654 HOMO: -6.74026 LUMO: 1.67622 factor:1 | -1 (1.18767) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.62337 HOMO: -6.76475 LUMO: 2.40277 factor:1 | -1 (1.26084) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.14289 HOMO: -6.65863 LUMO: 1.86670 factor:1 | -1 (0.74132) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.51496 HOMO: -6.50080 LUMO: 1.93201 factor:1 | -1 (1.36925) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.77865 HOMO: -6.34842 LUMO: 1.70888 factor:1 | -1 (2.10556) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.98790 HOMO: -6.60692 LUMO: 2.20140 factor:1 | -1 (1.89631) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.61189 HOMO: -6.74026 LUMO: 2.14970 factor:1 | -1 (1.27232) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.86825 HOMO: -6.63686 LUMO: 2.17419 factor:1 | -1 (2.01596) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.98287 HOMO: -6.81917 LUMO: 2.10072 factor:1 | -1 (1.90134) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.49322 HOMO: -6.92802 LUMO: 2.04358 factor:1 | -1 (1.39099) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.48845 HOMO: -6.56067 LUMO: -0.47620 factor:1 | -1 (1.39575) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.41879 HOMO: -6.56611 LUMO: -0.77008 factor:1 | -1 (1.46541) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.49959 HOMO: -6.78380 LUMO: -0.64763 factor:1 | -1 (2.38462) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.58626 HOMO: -6.51985 LUMO: -0.24490 factor:1 | -1 (2.29795) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.73620 HOMO: -6.52529 LUMO: -0.27483 factor:1 | -1 (2.14801) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.77799 HOMO: -7.10489 LUMO: -0.62586 factor:1 | -1 (2.10622) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.43230 HOMO: -7.18108 LUMO: 0.48980 factor:1 | -1 (2.45191) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.84327 HOMO: -7.14299 LUMO: -0.63947 factor:1 | -1 (2.04094) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.37588 HOMO: -6.70761 LUMO: -0.54423 factor:1 | -1 (1.50833) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.43419 HOMO: -7.32258 LUMO: -1.03675 factor:1 | -1 (1.45001) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.51915 HOMO: -6.65046 LUMO: -0.41361 factor:1 | -1 (1.36506) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.23035 HOMO: -6.76475 LUMO: -0.60137 factor:1 | -1 (1.65385) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.81380 HOMO: -6.77836 LUMO: -0.54423 factor:1 | -1 (2.07041) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.45841 HOMO: -7.52395 LUMO: 0.26395 factor:1 | -1 (1.42579) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.69975 HOMO: -6.93890 LUMO: -0.72382 factor:1 | -1 (1.18446) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.45477 HOMO: -6.72938 LUMO: -0.47348 factor:1 | -1 (1.42944) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.60867 HOMO: -6.66951 LUMO: -0.40817 factor:1 | -1 (1.27553) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.27404 HOMO: -6.60420 LUMO: -0.19320 factor:1 | -1 (2.61017) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.54278 HOMO: -6.67495 LUMO: -0.27211 factor:1 | -1 (2.34143) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.69641 HOMO: -7.23823 LUMO: -0.62858 factor:1 | -1 (2.18780) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.84360 HOMO: -7.27088 LUMO: 0.53334 factor:1 | -1 (2.04061) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.70558 HOMO: -7.20013 LUMO: 0.59049 factor:1 | -1 (2.17863) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.40652 HOMO: -6.60148 LUMO: -0.20953 factor:1 | -1 (1.47769) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.87470 HOMO: -6.69400 LUMO: -0.51974 factor:1 | -1 (2.00951) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.00730 HOMO: -7.40422 LUMO: -0.98777 factor:1 | -1 (1.87691) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.38837 HOMO: -6.88176 LUMO: -0.71022 factor:1 | -1 (1.49584) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.34170 HOMO: -6.86271 LUMO: -0.59321 factor:1 | -1 (1.54250) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.42769 HOMO: -6.73754 LUMO: -0.55239 factor:1 | -1 (1.45652) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.60675 HOMO: -6.71033 LUMO: 1.57010 factor:1 | -1 (2.27746) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.81437 HOMO: -6.69672 LUMO: 1.68711 factor:1 | -1 (2.06983) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.77655 HOMO: -6.67495 LUMO: 2.03813 factor:1 | -1 (2.10766) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.05734 HOMO: -6.54434 LUMO: 1.83677 factor:1 | -1 (0.82687) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.11902 HOMO: -6.57155 LUMO: 1.77146 factor:1 | -1 (0.76518) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57136 HOMO: -6.76747 LUMO: 1.87759 factor:1 | -1 (0.31285) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.43413 HOMO: -6.58243 LUMO: 1.61364 factor:1 | -1 (0.45008) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70157 HOMO: -6.61781 LUMO: 2.13881 factor:1 | -1 (0.18264) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.90530 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-0.02109) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61590 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-0.73169) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.32256 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-0.43835) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.32286 HOMO: -6.83278 LUMO: 1.91296 factor:1 | -1 (0.56134) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.32844 HOMO: -6.40012 LUMO: 1.95650 factor:1 | -1 (0.55577) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14242 HOMO: -6.50080 LUMO: 1.73337 factor:1 | 1 (-0.25821) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.99322 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-0.10901) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.22207 HOMO: -6.63686 LUMO: 2.20140 factor:1 | -1 (0.66213) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.33846 HOMO: -6.57427 LUMO: 1.87214 factor:1 | -1 (0.54575) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.19110 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-0.30689) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17722 HOMO: -6.63958 LUMO: 2.04902 factor:1 | 1 (-0.29301) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.02557 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-0.14136) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.26425 HOMO: -6.80557 LUMO: 2.23678 factor:1 | -1 (0.61996) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.19676 HOMO: -6.72938 LUMO: 2.28304 factor:1 | 1 (-0.31255) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.94447 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-1.06026) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.17552 HOMO: -6.95523 LUMO: 2.33474 factor:1 | 1 (-1.29132) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.06907 HOMO: -6.59876 LUMO: 2.30480 factor:1 | 1 (-1.18487) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.90021 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-0.01600) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01561 HOMO: -7.06408 LUMO: 1.99187 factor:1 | 1 (-0.13140) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.39316 HOMO: -6.95795 LUMO: 1.88847 factor:1 | 1 (-1.50895) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.05207 HOMO: -6.85455 LUMO: 1.63813 factor:1 | 1 (-1.16786) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.34079 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-0.45658) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.32166 HOMO: -6.91441 LUMO: 1.68983 factor:1 | 1 (-0.43745) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.29031 HOMO: -6.89809 LUMO: 2.23678 factor:1 | 1 (-0.40610) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.64528 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-0.76108) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.64387 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-0.75966) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.63356 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-0.74935) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.56169 HOMO: -6.94979 LUMO: 2.28031 factor:1 | 1 (-0.67748) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.75075 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-0.86655) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.72543 HOMO: -6.87360 LUMO: 2.40277 factor:1 | -1 (0.15878) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.08680 HOMO: -6.92802 LUMO: 1.89663 factor:1 | 1 (-0.20259) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.07806 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-0.19385) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61802 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-0.73381) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.39189 HOMO: -6.54978 LUMO: 1.93201 factor:1 | 1 (-0.50768) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.46705 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-0.58284) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50338 HOMO: -6.55794 LUMO: 1.89663 factor:1 | 1 (-0.61917) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.37259 HOMO: -6.07630 LUMO: 1.94289 factor:1 | -1 (1.51162) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.34846 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-0.46425) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.27950 HOMO: -6.63958 LUMO: -0.61770 factor:1 | 1 (-1.39529) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.08262 HOMO: -6.81101 LUMO: -0.57960 factor:1 | 1 (-1.19842) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30188 HOMO: -6.74298 LUMO: -0.57960 factor:1 | 1 (-0.41767) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.99265 HOMO: -6.63686 LUMO: -0.42994 factor:1 | 1 (-0.10844) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85828 HOMO: -6.60965 LUMO: -0.41089 factor:1 | -1 (0.02593) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.70827 HOMO: -6.60692 LUMO: -0.80274 factor:1 | -1 (1.17594) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.33518 HOMO: -6.58788 LUMO: -0.78097 factor:1 | 1 (-0.45097) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.51894 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-0.63473) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.62153 HOMO: -6.63141 LUMO: -0.40545 factor:1 | 1 (-0.73732) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.23651 HOMO: -6.62053 LUMO: -0.83811 factor:1 | 1 (-1.35230) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.95772 HOMO: -6.59604 LUMO: -0.35375 factor:1 | 1 (-1.07352) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.34931 HOMO: -6.34297 LUMO: -0.39729 factor:1 | 1 (-0.46510) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36041 HOMO: -6.67223 LUMO: 1.97827 factor:1 | 1 (-0.47620) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46777 HOMO: -6.40012 LUMO: 1.89935 factor:1 | -1 (0.41644) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.24041 HOMO: -6.74842 LUMO: 1.97283 factor:1 | 1 (-0.35620) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14253 HOMO: -6.76747 LUMO: 2.17147 factor:1 | 1 (-0.25832) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.50823 HOMO: -6.72121 LUMO: 1.55649 factor:1 | -1 (0.37598) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.40899 HOMO: -6.97700 LUMO: 2.04085 factor:1 | -1 (0.47522) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.57270 HOMO: -7.06680 LUMO: 2.04085 factor:1 | 1 (-1.68849) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.97362 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-1.08941) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.83024 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.94603) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.81624 HOMO: -6.72665 LUMO: 2.20140 factor:1 | 1 (-1.93204) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.40586 HOMO: -6.77291 LUMO: 2.34562 factor:1 | -1 (0.47835) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20250 HOMO: -6.73754 LUMO: 2.00276 factor:1 | 1 (-0.31829) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60290 HOMO: -7.04231 LUMO: 1.92112 factor:1 | -1 (0.28131) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.39741 HOMO: -6.83822 LUMO: 1.72248 factor:1 | 1 (-0.51321) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.28195 HOMO: -6.57971 LUMO: 2.16603 factor:1 | 1 (-1.39774) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.46345 HOMO: -6.80013 LUMO: 1.88575 factor:1 | 1 (-1.57924) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.54953 HOMO: -6.93618 LUMO: 2.18235 factor:1 | 1 (-0.66532) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.28562 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-1.40141) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.60164 HOMO: -7.06952 LUMO: 2.18507 factor:1 | 1 (-0.71743) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.41758 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-0.53337) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.19841 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-1.31420) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.83965 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-0.95545) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.54482 HOMO: -7.17292 LUMO: 1.90752 factor:1 | 1 (-0.66061) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.94965 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-0.06544) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.93248 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-0.04827) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.04886 HOMO: -6.85727 LUMO: 2.13609 factor:1 | 1 (-0.16466) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05474 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-0.17053) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.93931 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-0.05510) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.19093 HOMO: -6.67223 LUMO: 2.07351 factor:1 | 1 (-1.30672) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.51129 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-0.62709) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.51423 HOMO: -6.90897 LUMO: 2.28848 factor:1 | 1 (-0.63003) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69974 HOMO: -7.04231 LUMO: 1.70071 factor:1 | -1 (0.18447) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.04418 HOMO: -6.69944 LUMO: 1.94834 factor:1 | 1 (-1.15997) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30291 HOMO: -6.56067 LUMO: 2.20956 factor:1 | 1 (-0.41870) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.92093 HOMO: -6.65046 LUMO: 2.06807 factor:1 | 1 (-1.03673) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.20886 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-1.32465) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.36843 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-1.48422) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.76123 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-0.87702) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87215 HOMO: -6.85183 LUMO: 2.16058 factor:1 | -1 (0.01205) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.87800 HOMO: -6.54706 LUMO: 1.92384 factor:1 | 1 (-0.99379) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.79724 HOMO: -6.84366 LUMO: 2.48984 factor:1 | -1 (0.08697) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.73715 HOMO: -6.77291 LUMO: 2.46263 factor:1 | 1 (-0.85294) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.76556 HOMO: -7.01782 LUMO: 2.31025 factor:1 | 1 (-0.88135) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.84975 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-0.96554) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69588 HOMO: -6.64230 LUMO: 1.97283 factor:1 | -1 (0.18833) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.76787 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-0.88366) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.51984 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-0.63563) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.53419 HOMO: -7.17020 LUMO: 2.06807 factor:1 | -1 (0.35002) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.00905 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-0.12485) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.00541 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-0.12120) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.38572 HOMO: -6.83006 LUMO: 2.14970 factor:1 | -1 (0.49849) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.14954 HOMO: -6.92802 LUMO: 1.99187 factor:1 | -1 (1.73467) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.02753 HOMO: -6.69672 LUMO: 2.36739 factor:1 | 1 (-0.14332) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88380 HOMO: -7.13755 LUMO: 2.00276 factor:1 | -1 (0.00041) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.32526 HOMO: -6.92530 LUMO: 2.25582 factor:1 | -1 (0.55895) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01548 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-0.13127) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.78048 HOMO: -6.87904 LUMO: 1.60003 factor:1 | -1 (0.10373) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76238 HOMO: -6.62869 LUMO: 1.90480 factor:1 | -1 (0.12183) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.13011 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-1.24590) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.24772 HOMO: -6.74298 LUMO: 1.47486 factor:1 | 1 (-0.36352) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.04143 HOMO: -6.77019 LUMO: 1.90480 factor:1 | 1 (-1.15722) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.98486 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-0.10065) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91267 HOMO: -6.73482 LUMO: 2.08711 factor:1 | 1 (-0.02846) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.68166 HOMO: -6.46543 LUMO: 1.73881 factor:1 | 1 (-1.79745) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.12992 HOMO: -6.96067 LUMO: 2.26127 factor:1 | 1 (-1.24571) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.64881 HOMO: -6.67767 LUMO: 2.10616 factor:1 | 1 (-1.76460) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.10682 HOMO: -6.28855 LUMO: 2.35923 factor:1 | 1 (-1.22261) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.58945 HOMO: -6.80285 LUMO: 1.62724 factor:1 | 1 (-0.70524) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.58980 HOMO: -6.85455 LUMO: 2.23133 factor:1 | 1 (-0.70559) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.08772 HOMO: -6.51713 LUMO: 2.33474 factor:1 | 1 (-0.20351) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.69851 HOMO: -6.88176 LUMO: 2.15242 factor:1 | 1 (-0.81430) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.86062 HOMO: -6.54434 LUMO: 2.32113 factor:1 | -1 (0.02359) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.84051 HOMO: -6.62597 LUMO: 2.24222 factor:1 | -1 (0.04370) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.09793 HOMO: -6.74570 LUMO: 2.19868 factor:1 | 1 (-0.21372) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.97599 HOMO: -6.62869 LUMO: 1.98915 factor:1 | 1 (-0.09178) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89485 HOMO: -6.64502 LUMO: 2.13881 factor:1 | 1 (-0.01064) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06778 HOMO: -6.95795 LUMO: 1.82316 factor:1 | 1 (-0.18357) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01877 HOMO: -6.77291 LUMO: 1.36329 factor:1 | 1 (-0.13456) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76984 HOMO: -6.45726 LUMO: 1.73064 factor:1 | -1 (0.11437) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.92092 HOMO: -6.49264 LUMO: 1.77418 factor:1 | 1 (-0.03671) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.63718 HOMO: -6.60420 LUMO: 2.20956 factor:1 | -1 (0.24702) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77204 HOMO: -6.56067 LUMO: 2.05718 factor:1 | -1 (0.11217) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.35545 HOMO: -6.62597 LUMO: 1.70343 factor:1 | -1 (1.52876) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.85269 HOMO: -6.69400 LUMO: 2.16875 factor:1 | 1 (-0.96848) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.87609 HOMO: -6.63958 LUMO: 2.11977 factor:1 | 1 (-0.99188) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.77575 HOMO: -6.92802 LUMO: 1.82044 factor:1 | -1 (1.10846) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.20256 HOMO: -6.56339 LUMO: 2.30480 factor:1 | -1 (0.68165) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.25694 HOMO: -6.63958 LUMO: 1.91024 factor:1 | 1 (-1.37273) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.35542 HOMO: -6.93074 LUMO: 2.05446 factor:1 | 1 (-1.47121) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.85875 HOMO: -6.61509 LUMO: 2.03813 factor:1 | 1 (-1.97454) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.56982 HOMO: -6.61237 LUMO: 1.91296 factor:1 | 1 (-1.68561) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.27461 HOMO: -6.86815 LUMO: 1.95378 factor:1 | 1 (-0.39040) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88415 HOMO: -6.63686 LUMO: 1.70888 factor:1 | -1 (0.00005) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.83476 HOMO: -6.57971 LUMO: 2.20140 factor:1 | -1 (0.04944) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.31880 HOMO: -6.41100 LUMO: 1.96738 factor:1 | 1 (-0.43459) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87308 HOMO: -6.90081 LUMO: 1.65989 factor:1 | -1 (0.01113) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81719 HOMO: -6.68312 LUMO: 1.97827 factor:1 | -1 (0.06702) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.95030 HOMO: -6.65318 LUMO: 2.10888 factor:1 | 1 (-0.06610) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61810 HOMO: -6.62053 LUMO: 2.28848 factor:1 | 1 (-0.73389) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.74714 HOMO: -6.65863 LUMO: 2.29664 factor:1 | -1 (0.13706) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.44647 HOMO: -6.63958 LUMO: 2.07623 factor:1 | 1 (-1.56226) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.30192 HOMO: -6.58243 LUMO: 2.20684 factor:1 | 1 (-1.41771) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.81203 HOMO: -6.59332 LUMO: 2.05174 factor:1 | 1 (-0.92783) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96301 HOMO: -6.95251 LUMO: 2.20140 factor:1 | 1 (-0.07880) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.86390 HOMO: -6.84638 LUMO: 2.39732 factor:1 | 1 (-0.97969) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.20078 HOMO: -6.86815 LUMO: 2.47896 factor:1 | 1 (-1.31657) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.52580 HOMO: -7.00693 LUMO: 2.43270 factor:1 | 1 (-0.64159) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.54095 HOMO: -6.58788 LUMO: 2.30208 factor:1 | 1 (-0.65675) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.91030 HOMO: -6.63958 LUMO: 2.28031 factor:1 | 1 (-1.02609) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.91674 HOMO: -6.74570 LUMO: 2.28304 factor:1 | 1 (-1.03254) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.98486 HOMO: -6.78380 LUMO: 2.16331 factor:1 | 1 (-0.10065) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.29735 HOMO: -6.52529 LUMO: 2.05718 factor:1 | 1 (-1.41314) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.57720 HOMO: -6.41644 LUMO: 1.65445 factor:1 | 1 (-0.69299) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.52457 HOMO: -6.34570 LUMO: 1.22451 factor:1 | 1 (-0.64037) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.86817 HOMO: -6.14433 LUMO: 1.85582 factor:1 | 1 (-0.98396) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.42028 HOMO: -6.62053 LUMO: 1.92112 factor:1 | -1 (0.46393) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.51561 HOMO: -6.63414 LUMO: 1.61908 factor:1 | -1 (1.36860) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.07045 HOMO: -6.75931 LUMO: 1.87214 factor:1 | -1 (0.81376) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.13884 HOMO: -6.55794 LUMO: 1.77418 factor:1 | 1 (-1.25464) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.15300 HOMO: -6.52801 LUMO: 1.82044 factor:1 | 1 (-0.26879) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.02703 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-1.14282) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.13491 HOMO: -6.93890 LUMO: 1.81228 factor:1 | 1 (-0.25070) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.48446 HOMO: -6.85455 LUMO: 1.75513 factor:1 | 1 (-0.60026) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.61857 HOMO: -6.86815 LUMO: 1.64629 factor:1 | -1 (0.26564) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.75225 HOMO: -6.98516 LUMO: 1.84765 factor:1 | 1 (-0.86804) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.53881 HOMO: -6.04637 LUMO: 1.94017 factor:1 | 1 (-0.65460) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.66946 HOMO: -6.86271 LUMO: 2.11977 factor:1 | -1 (0.21475) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.39054 HOMO: -6.72938 LUMO: 2.11160 factor:1 | -1 (0.49367) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.98159 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-1.09738) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87452 HOMO: -6.18515 LUMO: 2.04630 factor:1 | -1 (0.00969) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36873 HOMO: -6.60965 LUMO: 2.17147 factor:1 | 1 (-0.48453) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80481 HOMO: -6.87360 LUMO: 2.35378 factor:1 | -1 (0.07940) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60643 HOMO: -6.72938 LUMO: 2.20140 factor:1 | -1 (0.27777) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.65695 HOMO: -6.88448 LUMO: 2.54154 factor:1 | -1 (1.22726) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79799 HOMO: -6.87087 LUMO: 2.16058 factor:1 | 1 (-0.91379) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.08130 HOMO: -7.11306 LUMO: 2.04085 factor:1 | 1 (-0.19709) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.63021 HOMO: -6.66951 LUMO: 1.68438 factor:1 | 1 (-0.74600) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.38437 HOMO: -7.08312 LUMO: 2.19324 factor:1 | -1 (1.49984) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.10922 HOMO: -6.69128 LUMO: 2.13881 factor:1 | 1 (-0.22501) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14674 HOMO: -6.80285 LUMO: 2.16603 factor:1 | 1 (-0.26254) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.17071 HOMO: -6.82189 LUMO: 2.46807 factor:1 | -1 (1.71350) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.93507 HOMO: -6.78652 LUMO: 2.12521 factor:1 | 1 (-0.05086) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23368 HOMO: -6.47903 LUMO: 1.70071 factor:1 | 1 (-0.34948) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17439 HOMO: -6.37019 LUMO: 1.24356 factor:1 | 1 (-0.29018) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.16519 HOMO: -6.69400 LUMO: 1.67350 factor:1 | 1 (-0.28098) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.67919 HOMO: -7.51851 LUMO: 0.27756 factor:1 | -1 (2.20502) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57460 HOMO: -6.95795 LUMO: -0.72110 factor:1 | -1 (0.30961) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.61140 HOMO: -6.88720 LUMO: -0.67484 factor:1 | -1 (1.27281) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.90023 HOMO: -6.83550 LUMO: -0.57144 factor:1 | -1 (1.98398) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88843 HOMO: -6.80285 LUMO: -0.57144 factor:1 | 1 (-0.00422) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.19913 HOMO: -6.76475 LUMO: -0.53062 factor:1 | 1 (-0.31492) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.75618 HOMO: -6.66951 LUMO: 1.74969 factor:1 | -1 (0.12803) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.92394 HOMO: -6.53345 LUMO: 1.89935 factor:1 | 1 (-0.03973) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.42717 HOMO: -6.65046 LUMO: 2.01364 factor:1 | -1 (0.45704) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.50350 HOMO: -6.64230 LUMO: 2.11977 factor:1 | -1 (1.38071) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.55722 HOMO: -6.44910 LUMO: 2.13337 factor:1 | -1 (1.32699) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.22442 HOMO: -7.05591 LUMO: 1.98915 factor:1 | -1 (1.65979) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.31417 HOMO: -7.02326 LUMO: 2.49256 factor:1 | -1 (1.57004) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52616 HOMO: -6.32937 LUMO: 2.51161 factor:1 | -1 (0.35805) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.67061 HOMO: -6.96067 LUMO: 2.20140 factor:1 | -1 (1.21360) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.37283 HOMO: -6.97972 LUMO: 2.55243 factor:1 | -1 (1.51137) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.92392 HOMO: -6.72665 LUMO: 2.46535 factor:1 | -1 (0.96029) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.71513 HOMO: -6.41917 LUMO: 2.35106 factor:1 | 1 (-0.83093) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05575 HOMO: -6.75114 LUMO: 2.32929 factor:1 | 1 (-0.17154) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.81818 HOMO: -6.91713 LUMO: 2.27215 factor:1 | 1 (-0.93398) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.29227 HOMO: -6.54978 LUMO: 2.00276 factor:1 | 1 (-0.40806) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.08797 HOMO: -6.62325 LUMO: 2.05990 factor:1 | 1 (-0.20376) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.19039 HOMO: -6.86271 LUMO: 2.14970 factor:1 | 1 (-0.30618) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.74292 HOMO: -6.77564 LUMO: 2.25855 factor:1 | 1 (-0.85871) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14408 HOMO: -6.71305 LUMO: 1.94561 factor:1 | 1 (-0.25987) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14500 HOMO: -6.75659 LUMO: 1.94561 factor:1 | 1 (-0.26079) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80105 HOMO: -6.94979 LUMO: 2.33474 factor:1 | -1 (0.08316) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.92046 HOMO: -6.85727 LUMO: 2.50345 factor:1 | -1 (0.96375) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.03678 HOMO: -6.87360 LUMO: 2.43270 factor:1 | 1 (-0.15257) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81645 HOMO: -6.57427 LUMO: 2.46807 factor:1 | -1 (0.06776) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11678 HOMO: -7.16204 LUMO: 2.15242 factor:1 | 1 (-0.23258) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.27583 HOMO: -6.62869 LUMO: 2.11432 factor:1 | 1 (-0.39163) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11510 HOMO: -7.05591 LUMO: 2.26671 factor:1 | 1 (-0.23089) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.07253 HOMO: -7.13483 LUMO: 1.47758 factor:1 | -1 (1.81168) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.47333 HOMO: -6.72938 LUMO: 1.57282 factor:1 | 1 (-0.58913) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.31834 HOMO: -6.17426 LUMO: 1.81228 factor:1 | 1 (-0.43413) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81762 HOMO: -6.65318 LUMO: 1.93473 factor:1 | -1 (0.06659) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.04264 HOMO: -6.18515 LUMO: 2.01364 factor:1 | -1 (0.84157) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.27992 HOMO: -7.05591 LUMO: 2.13337 factor:1 | 1 (-0.39571) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.02307 HOMO: -6.90897 LUMO: 2.29664 factor:1 | 1 (-0.13886) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01436 HOMO: -7.11034 LUMO: 2.17147 factor:1 | 1 (-0.13015) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.10908 HOMO: -6.82734 LUMO: 2.26671 factor:1 | 1 (-0.22487) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62080 HOMO: -6.34842 LUMO: 2.34562 factor:1 | -1 (0.26341) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.99608 HOMO: -6.62053 LUMO: 2.22861 factor:1 | -1 (0.88813) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.32343 HOMO: -6.80557 LUMO: 2.07079 factor:1 | 1 (-0.43922) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45862 HOMO: -6.60692 LUMO: 2.46263 factor:1 | -1 (0.42559) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23709 HOMO: -7.02054 LUMO: 2.08711 factor:1 | 1 (-0.35288) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57179 HOMO: -6.78652 LUMO: 2.02453 factor:1 | -1 (0.31241) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62692 HOMO: -6.51168 LUMO: 2.06534 factor:1 | -1 (0.25728) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.66762 HOMO: -6.50080 LUMO: 2.01636 factor:1 | 1 (-0.78342) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.33769 HOMO: -6.54434 LUMO: 1.84493 factor:1 | 1 (-0.45348) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.65840 HOMO: -6.47087 LUMO: 1.76330 factor:1 | 1 (-0.77419) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.84625 HOMO: -6.78924 LUMO: 2.39460 factor:1 | -1 (0.03796) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.51625 HOMO: -6.59876 LUMO: 1.84493 factor:1 | 1 (-0.63204) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79691 HOMO: -6.41644 LUMO: 2.05174 factor:1 | 1 (-0.91270) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05637 HOMO: -6.52257 LUMO: 2.11160 factor:1 | 1 (-0.17217) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.95108 HOMO: -6.90897 LUMO: 2.34018 factor:1 | 1 (-1.06688) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.98037 HOMO: -6.97428 LUMO: 1.86126 factor:1 | 1 (-0.09617) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.92230 HOMO: -7.13483 LUMO: 2.14698 factor:1 | 1 (-1.03809) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.69157 HOMO: -7.16748 LUMO: 2.31841 factor:1 | 1 (-0.80736) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.87253 HOMO: -6.87087 LUMO: 2.38916 factor:1 | -1 (0.01167) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.53285 HOMO: -6.93074 LUMO: 2.42181 factor:1 | 1 (-0.64864) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01246 HOMO: -6.90081 LUMO: 2.00276 factor:1 | 1 (-0.12825) | 1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.58158 HOMO: -6.99333 LUMO: 2.03541 factor:1 | 1 (-0.69737) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.74490 HOMO: -6.89264 LUMO: 1.57554 factor:1 | 1 (-0.86070) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.63998 HOMO: -6.48175 LUMO: 1.85854 factor:1 | 1 (-0.75577) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.26777 HOMO: -6.69400 LUMO: 1.62452 factor:1 | -1 (1.61644) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.63481 HOMO: -6.50896 LUMO: 1.88303 factor:1 | 1 (-0.75060) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64986 HOMO: -6.60420 LUMO: 2.05990 factor:1 | -1 (0.23434) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06514 HOMO: -7.14299 LUMO: 2.07351 factor:1 | 1 (-0.18093) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.72399 HOMO: -7.06408 LUMO: 1.81228 factor:1 | -1 (0.16022) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11714 HOMO: -6.67495 LUMO: 1.79595 factor:1 | 1 (-0.23293) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.13058 HOMO: -6.45182 LUMO: 2.15786 factor:1 | 1 (-0.24637) | -1 | -1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96761 HOMO: -6.93346 LUMO: 2.45719 factor:1 | 1 (-0.08340) | 1 | 1 |
| G: -6695.51851 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06587 HOMO: -6.50080 LUMO: 2.08167 factor:1 | 1 (-0.18166) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.28364 HOMO: -6.83550 LUMO: -0.67484 factor:1 | 1 (-0.39944) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.22283 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-0.33862) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30511 HOMO: -6.79740 LUMO: 1.91296 factor:1 | 1 (-0.42091) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.37377 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-0.48956) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89798 HOMO: -6.62597 LUMO: -0.44082 factor:1 | 1 (-0.01377) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.44737 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-0.56317) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.29942 HOMO: -6.51168 LUMO: -0.23130 factor:1 | -1 (1.58479) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89858 HOMO: -7.14027 LUMO: 0.49797 factor:1 | 1 (-0.01437) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52850 HOMO: -7.55660 LUMO: 0.24762 factor:1 | -1 (0.35571) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.60209 HOMO: -6.88992 LUMO: -0.64763 factor:1 | -1 (1.28212) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.37032 HOMO: -6.72665 LUMO: -0.45987 factor:1 | -1 (0.51389) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88788 HOMO: -6.72121 LUMO: -0.58232 factor:1 | 1 (-0.00367) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.38795 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-0.50374) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.37668 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-0.49247) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.67181 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-0.78761) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85602 HOMO: -6.73210 LUMO: -0.51430 factor:1 | -1 (0.02819) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.72486 HOMO: -6.77019 LUMO: -0.62858 factor:1 | -1 (0.15935) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.78096 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-0.89675) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.86829 HOMO: -6.79740 LUMO: -0.55511 factor:1 | -1 (0.01592) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.64338 HOMO: -6.79740 LUMO: -0.67756 factor:1 | 1 (-0.75917) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59332 HOMO: -6.75114 LUMO: -0.55239 factor:1 | -1 (0.29089) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.65383 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-0.76962) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.12617 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-0.24196) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.99953 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-0.11532) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.34129 HOMO: -7.22462 LUMO: 0.52518 factor:1 | -1 (0.54292) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.00239 HOMO: -6.59332 LUMO: -0.27211 factor:1 | 1 (-0.11818) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.44245 HOMO: -6.57427 LUMO: -0.16871 factor:1 | 1 (-0.55824) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.46150 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-0.57729) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.68420 HOMO: -6.72121 LUMO: 2.00004 factor:1 | 1 (-0.79999) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.42294 HOMO: -6.61509 LUMO: 1.55921 factor:1 | 1 (-0.53873) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.43369 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-0.54948) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.70158 HOMO: -6.66135 LUMO: 2.02181 factor:1 | 1 (-0.81738) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.46052 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-0.57631) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64154 HOMO: -6.66679 LUMO: 1.98371 factor:1 | -1 (0.24267) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.20498 HOMO: -6.67495 LUMO: 2.04085 factor:1 | 1 (-0.32077) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.31916 HOMO: -6.89809 LUMO: 1.95106 factor:1 | -1 (0.56504) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.65620 HOMO: -6.50352 LUMO: 1.88847 factor:1 | -1 (0.22800) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.68316 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-0.79895) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.87035 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-0.98614) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81776 HOMO: -6.69672 LUMO: 2.37283 factor:1 | -1 (0.06645) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46567 HOMO: -6.65591 LUMO: 2.20684 factor:1 | -1 (0.41854) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.11546 HOMO: -6.23957 LUMO: 1.78507 factor:1 | -1 (0.76875) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.47336 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-0.58915) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06737 HOMO: -6.53617 LUMO: 1.75241 factor:1 | 1 (-0.18316) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.73215 HOMO: -6.60420 LUMO: 1.78779 factor:1 | -1 (0.15206) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58045 HOMO: -7.40422 LUMO: -0.97145 factor:1 | -1 (0.30376) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.13409 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-0.24988) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.21979 HOMO: -6.68040 LUMO: -0.47076 factor:1 | -1 (0.66442) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23001 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-0.34580) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91504 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-0.03083) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60785 HOMO: -7.18653 LUMO: 0.59321 factor:1 | -1 (0.27636) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50901 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-0.62480) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.43694 HOMO: -6.63414 LUMO: -0.25034 factor:1 | -1 (1.44726) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.64148 HOMO: -7.20285 LUMO: 0.53879 factor:1 | -1 (0.24273) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06745 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-0.18324) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.52240 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-0.63819) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.99615 HOMO: -6.90897 LUMO: 1.91296 factor:1 | 1 (-1.11194) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.96638 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-1.08217) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.67364 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-0.78943) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.03794 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-1.15374) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.34053 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-1.45633) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.76482 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-0.88061) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.23849 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-1.35428) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.63066 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-1.74645) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.26897 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-1.38476) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76568 HOMO: -6.84911 LUMO: 1.89935 factor:1 | -1 (0.11853) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.55027 HOMO: -6.22052 LUMO: 1.57282 factor:1 | -1 (0.33394) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58080 HOMO: -6.51168 LUMO: 2.10072 factor:1 | -1 (0.30341) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.98884 HOMO: -7.03686 LUMO: 2.12249 factor:1 | -1 (0.89536) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79388 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-0.90968) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89009 HOMO: -6.75387 LUMO: 1.72248 factor:1 | 1 (-0.00588) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.38101 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-0.49680) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.28739 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-1.40318) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.73369 HOMO: -6.80557 LUMO: 2.02725 factor:1 | 1 (-0.84949) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.37131 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-1.48710) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.40278 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-0.51857) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.78635 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-0.90214) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.00843 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-0.12422) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85730 HOMO: -6.71305 LUMO: -0.49525 factor:1 | -1 (0.02691) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.74374 HOMO: -6.60692 LUMO: -0.22313 factor:1 | -1 (0.14047) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.49966 HOMO: -7.20013 LUMO: 0.55239 factor:1 | -1 (0.38455) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52156 HOMO: -6.60420 LUMO: -0.28028 factor:1 | -1 (0.36265) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69710 HOMO: -6.69128 LUMO: -0.30477 factor:1 | -1 (0.18711) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.56265 HOMO: -6.65591 LUMO: -0.25579 factor:1 | -1 (0.32156) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.08860 HOMO: -6.69128 LUMO: 1.70888 factor:1 | -1 (0.79561) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.91175 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-0.02754) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.04214 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-0.15793) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70782 HOMO: -6.58788 LUMO: 1.79051 factor:1 | -1 (0.17638) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.52477 HOMO: -6.64230 LUMO: 2.16058 factor:1 | -1 (0.35944) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.56113 HOMO: -6.58788 LUMO: 2.10616 factor:1 | -1 (0.32308) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.96860 HOMO: -7.01782 LUMO: 2.13609 factor:1 | -1 (0.91561) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.39513 HOMO: -6.31304 LUMO: 2.31841 factor:1 | 1 (-0.51092) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.30302 HOMO: -6.94979 LUMO: 2.07895 factor:1 | 1 (-0.41881) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.71576 HOMO: -6.88992 LUMO: 2.28031 factor:1 | 1 (-0.83155) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.99762 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-1.11341) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.71475 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-1.83054) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.00222 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-1.11801) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.56903 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-1.68482) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14680 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-0.26259) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.72518 HOMO: -6.31304 LUMO: 2.18507 factor:1 | 1 (-0.84097) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.71633 HOMO: -6.18243 LUMO: 2.01636 factor:1 | 1 (-0.83212) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50887 HOMO: -6.99877 LUMO: 2.14970 factor:1 | 1 (-0.62466) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79271 HOMO: -6.72665 LUMO: 2.07079 factor:1 | 1 (-0.90851) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.18244 HOMO: -6.36202 LUMO: 2.17419 factor:1 | 1 (-1.29823) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.10341 HOMO: -6.78652 LUMO: 2.05718 factor:1 | 1 (-1.21921) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.09871 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-1.21450) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.03749 HOMO: -6.62053 LUMO: 1.89391 factor:1 | 1 (-0.15328) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06182 HOMO: -6.58788 LUMO: 1.83133 factor:1 | 1 (-0.17761) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.56015 HOMO: -7.08584 LUMO: 1.91568 factor:1 | -1 (0.32406) | 1 | 1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.71044 HOMO: -6.56883 LUMO: 1.81228 factor:1 | -1 (0.17377) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.06837 HOMO: -6.66135 LUMO: 1.92384 factor:1 | 1 (-0.18417) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.00930 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-0.12509) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58905 HOMO: -6.71305 LUMO: 1.91840 factor:1 | -1 (0.29516) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62431 HOMO: -6.44094 LUMO: 1.74425 factor:1 | -1 (0.25990) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77846 HOMO: -6.51985 LUMO: 1.84221 factor:1 | -1 (0.10574) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.12867 HOMO: -6.63414 LUMO: -0.24762 factor:1 | 1 (-1.24446) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.09098 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-1.20677) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.49044 HOMO: -7.19741 LUMO: 0.58232 factor:1 | 1 (-1.60623) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.65080 HOMO: -6.77019 LUMO: -0.56872 factor:1 | 1 (-1.76659) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.52835 HOMO: -7.46136 LUMO: 0.28844 factor:1 | 1 (-1.64414) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.36824 HOMO: -6.60420 LUMO: -0.54151 factor:1 | 1 (-1.48403) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.68802 HOMO: -6.53890 LUMO: -0.46531 factor:1 | 1 (-1.80382) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.67687 HOMO: -6.81645 LUMO: -0.57144 factor:1 | 1 (-1.79266) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.73821 HOMO: -7.48041 LUMO: 0.28572 factor:1 | 1 (-0.85400) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.48190 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-1.59769) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.88447 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-1.00026) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.04639 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-0.16218) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05444 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-0.17023) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58086 HOMO: -7.12394 LUMO: 0.53334 factor:1 | -1 (0.30335) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68521 HOMO: -6.53617 LUMO: -0.25579 factor:1 | -1 (0.19900) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.53095 HOMO: -6.50896 LUMO: -0.25034 factor:1 | -1 (0.35326) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.34662 HOMO: -7.17564 LUMO: -0.68573 factor:1 | -1 (0.53759) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17540 HOMO: -6.53617 LUMO: -0.30749 factor:1 | 1 (-0.29119) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.17830 HOMO: -6.55522 LUMO: -0.30749 factor:1 | 1 (-1.29409) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.32792 HOMO: -7.05591 LUMO: -0.71022 factor:1 | 1 (-0.44371) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.05574 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-1.17153) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.31724 HOMO: -6.78380 LUMO: -0.67756 factor:1 | 1 (-1.43303) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.46084 HOMO: -6.62325 LUMO: 2.02725 factor:1 | 1 (-0.57664) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.31924 HOMO: -6.63414 LUMO: 1.91296 factor:1 | 1 (-0.43503) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.01220 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-1.12799) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.50452 HOMO: -6.66407 LUMO: 1.95650 factor:1 | 1 (-0.62031) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.66818 HOMO: -6.61237 LUMO: 2.11432 factor:1 | -1 (0.21603) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.72578 HOMO: -6.62053 LUMO: 2.09256 factor:1 | -1 (0.15842) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.63538 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-0.75117) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.04173 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-1.15752) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79759 HOMO: -6.85183 LUMO: 2.12793 factor:1 | 1 (-0.91338) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76706 HOMO: -6.81101 LUMO: 1.83949 factor:1 | -1 (0.11715) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59792 HOMO: -6.98788 LUMO: 2.16058 factor:1 | -1 (0.28629) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.70390 HOMO: -6.62869 LUMO: 2.00820 factor:1 | 1 (-0.81969) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.78368 HOMO: -6.34025 LUMO: 2.25855 factor:1 | 1 (-0.89947) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.42952 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-0.54532) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.76266 HOMO: -6.89264 LUMO: 2.27487 factor:1 | -1 (1.12154) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.66984 HOMO: -6.53073 LUMO: 2.20684 factor:1 | -1 (0.21437) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.37815 HOMO: -6.83278 LUMO: 1.53744 factor:1 | 1 (-0.49394) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.51881 HOMO: -6.41917 LUMO: 1.82316 factor:1 | -1 (0.36539) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.91049 HOMO: -6.56339 LUMO: 1.63813 factor:1 | 1 (-1.02628) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.07384 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-1.18963) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45810 HOMO: -6.63141 LUMO: 1.92112 factor:1 | -1 (0.42610) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61617 HOMO: -6.83822 LUMO: 1.88847 factor:1 | 1 (-0.73196) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.04017 HOMO: -6.84638 LUMO: 1.90480 factor:1 | -1 (0.84404) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.30123 HOMO: -6.82462 LUMO: 1.70888 factor:1 | -1 (0.58298) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.87318 HOMO: -6.82734 LUMO: 2.12521 factor:1 | 1 (-0.98897) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.45252 HOMO: -6.94435 LUMO: 1.87214 factor:1 | 1 (-0.56831) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.04880 HOMO: -6.98516 LUMO: 2.51433 factor:1 | 1 (-1.16459) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.59189 HOMO: -6.74026 LUMO: 2.15514 factor:1 | 1 (-0.70769) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.77973 HOMO: -6.93618 LUMO: 2.54426 factor:1 | 1 (-0.89553) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.17442 HOMO: -6.28583 LUMO: 2.53610 factor:1 | 1 (-0.29021) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57982 HOMO: -6.56883 LUMO: 1.94834 factor:1 | -1 (0.30439) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.68630 HOMO: -7.08584 LUMO: 1.99187 factor:1 | -1 (0.19791) | 1 | 1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.45831 HOMO: -6.19059 LUMO: 1.99732 factor:1 | 1 (-0.57411) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.28711 HOMO: -6.78108 LUMO: 2.03813 factor:1 | -1 (0.59710) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58747 HOMO: -6.82189 LUMO: 1.77418 factor:1 | -1 (0.29674) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.86653 HOMO: -6.45454 LUMO: 1.78779 factor:1 | -1 (1.01768) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88976 HOMO: -6.84366 LUMO: 1.77690 factor:1 | 1 (-0.00555) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.37310 HOMO: -6.74026 LUMO: 1.67622 factor:1 | -1 (0.51111) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96312 HOMO: -6.76475 LUMO: 2.40277 factor:1 | 1 (-0.07891) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.02123 HOMO: -6.65863 LUMO: 1.86670 factor:1 | -1 (0.86298) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.71464 HOMO: -6.50080 LUMO: 1.93201 factor:1 | -1 (1.16957) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69629 HOMO: -6.34842 LUMO: 1.70888 factor:1 | -1 (0.18792) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.92206 HOMO: -6.60692 LUMO: 2.20140 factor:1 | 1 (-0.03785) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27024 HOMO: -6.74026 LUMO: 2.14970 factor:1 | -1 (0.61397) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.98675 HOMO: -6.63686 LUMO: 2.17419 factor:1 | -1 (0.89746) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69751 HOMO: -6.81917 LUMO: 2.10072 factor:1 | -1 (0.18670) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05039 HOMO: -6.92802 LUMO: 2.04358 factor:1 | 1 (-0.16618) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.62327 HOMO: -6.56067 LUMO: -0.47620 factor:1 | 1 (-0.73906) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.88383 HOMO: -6.56611 LUMO: -0.77008 factor:1 | -1 (0.00038) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.55737 HOMO: -6.78380 LUMO: -0.64763 factor:1 | -1 (0.32684) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.26983 HOMO: -6.51985 LUMO: -0.24490 factor:1 | -1 (0.61438) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.59345 HOMO: -6.52529 LUMO: -0.27483 factor:1 | -1 (0.29075) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46572 HOMO: -7.10489 LUMO: -0.62586 factor:1 | -1 (0.41848) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.70061 HOMO: -7.18108 LUMO: 0.48980 factor:1 | -1 (0.18360) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81909 HOMO: -7.14299 LUMO: -0.63947 factor:1 | -1 (0.06512) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.02703 HOMO: -6.70761 LUMO: -0.54423 factor:1 | 1 (-1.14282) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.29177 HOMO: -7.32258 LUMO: -1.03675 factor:1 | 1 (-1.40756) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61236 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-0.72815) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.36473 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-0.48053) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77212 HOMO: -6.77836 LUMO: -0.54423 factor:1 | -1 (0.11208) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.24160 HOMO: -7.52395 LUMO: 0.26395 factor:1 | 1 (-0.35739) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.66635 HOMO: -6.93890 LUMO: -0.72382 factor:1 | -1 (0.21785) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27451 HOMO: -6.72938 LUMO: -0.47348 factor:1 | -1 (0.60970) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.05463 HOMO: -6.66951 LUMO: -0.40817 factor:1 | 1 (-0.17042) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58706 HOMO: -6.60420 LUMO: -0.19320 factor:1 | -1 (0.29715) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.81041 HOMO: -6.67495 LUMO: -0.27211 factor:1 | -1 (0.07380) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.75579 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-0.87158) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.23822 HOMO: -7.27088 LUMO: 0.53334 factor:1 | 1 (-1.35401) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.67630 HOMO: -7.20013 LUMO: 0.59049 factor:1 | 1 (-0.79210) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.47872 HOMO: -6.60148 LUMO: -0.20953 factor:1 | 1 (-0.59451) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.69481 HOMO: -6.69400 LUMO: -0.51974 factor:1 | 1 (-0.81060) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.27119 HOMO: -7.40422 LUMO: -0.98777 factor:1 | -1 (0.61302) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.04114 HOMO: -6.88176 LUMO: -0.71022 factor:1 | -1 (0.84306) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.31160 HOMO: -6.86271 LUMO: -0.59321 factor:1 | -1 (0.57261) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.42537 HOMO: -6.73754 LUMO: -0.55239 factor:1 | -1 (0.45884) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.24509 HOMO: -6.71033 LUMO: 1.57010 factor:1 | -1 (0.63911) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.26678 HOMO: -6.69672 LUMO: 1.68711 factor:1 | -1 (0.61743) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.22085 HOMO: -6.67495 LUMO: 2.03813 factor:1 | -1 (0.66336) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.79440 HOMO: -6.54434 LUMO: 1.83677 factor:1 | 1 (-0.91019) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80168 HOMO: -6.57155 LUMO: 1.77146 factor:1 | -1 (0.08253) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.37692 HOMO: -6.76747 LUMO: 1.87759 factor:1 | 1 (-1.49271) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.64773 HOMO: -6.58243 LUMO: 1.61364 factor:1 | 1 (-0.76352) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.39358 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-0.50937) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.70537 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-0.82116) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.38289 HOMO: -7.01237 LUMO: 1.95922 factor:1 | -1 (0.50132) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.43651 HOMO: -7.03959 LUMO: 2.16875 factor:1 | -1 (1.44770) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.10047 HOMO: -6.83278 LUMO: 1.91296 factor:1 | -1 (0.78374) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.40044 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-0.51623) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.56842 HOMO: -6.50080 LUMO: 1.73337 factor:1 | -1 (0.31579) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.37214 HOMO: -6.95795 LUMO: 2.28848 factor:1 | -1 (0.51206) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.12261 HOMO: -6.63686 LUMO: 2.20140 factor:1 | 1 (-0.23840) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.18441 HOMO: -6.57427 LUMO: 1.87214 factor:1 | -1 (0.69980) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.38574 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-0.50153) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.49870 HOMO: -6.63958 LUMO: 2.04902 factor:1 | -1 (0.38550) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.32858 HOMO: -6.70216 LUMO: 1.93201 factor:1 | -1 (0.55563) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.11670 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-0.23249) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.55808 HOMO: -6.72938 LUMO: 2.28304 factor:1 | -1 (0.32613) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.15156 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-0.26735) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.25738 HOMO: -6.95523 LUMO: 2.33474 factor:1 | -1 (2.62682) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.97332 HOMO: -6.59876 LUMO: 2.30480 factor:1 | -1 (1.91089) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.61589 HOMO: -6.87360 LUMO: 1.75786 factor:1 | -1 (2.26831) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.92113 HOMO: -7.06408 LUMO: 1.99187 factor:1 | 1 (-0.03693) | 1 | 1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45740 HOMO: -6.95795 LUMO: 1.88847 factor:1 | -1 (0.42681) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.13640 HOMO: -6.85455 LUMO: 1.63813 factor:1 | 1 (-0.25220) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.99145 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-0.10724) | 1 | 1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.61928 HOMO: -6.91441 LUMO: 1.68983 factor:1 | -1 (0.26493) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.36964 HOMO: -6.89809 LUMO: 2.23678 factor:1 | -1 (0.51457) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.02307 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-0.13886) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.13224 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-0.24803) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.04271 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-0.15851) | 1 | 1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.10205 HOMO: -6.94979 LUMO: 2.28031 factor:1 | -1 (1.78216) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76168 HOMO: -6.60965 LUMO: 2.20412 factor:1 | -1 (0.12253) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.64851 HOMO: -6.87360 LUMO: 2.40277 factor:1 | -1 (1.23570) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.11824 HOMO: -6.92802 LUMO: 1.89663 factor:1 | 1 (-1.23404) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.23907 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-0.35486) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.98208 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-1.09787) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.07852 HOMO: -6.54978 LUMO: 1.93201 factor:1 | 1 (-0.19432) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12961.09800 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-1.21379) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.22089 HOMO: -6.55794 LUMO: 1.89663 factor:1 | 1 (-0.33669) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.69873 HOMO: -6.07630 LUMO: 1.94289 factor:1 | 1 (-0.81452) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96549 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-0.08128) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.20243 HOMO: -6.63958 LUMO: -0.61770 factor:1 | -1 (0.68178) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.80620 HOMO: -6.81101 LUMO: -0.57960 factor:1 | -1 (1.07801) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58086 HOMO: -6.74298 LUMO: -0.57960 factor:1 | -1 (0.30335) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.93403 HOMO: -6.63686 LUMO: -0.42994 factor:1 | 1 (-0.04982) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.57238 HOMO: -6.60965 LUMO: -0.41089 factor:1 | 1 (-0.68818) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.82689 HOMO: -6.60692 LUMO: -0.80274 factor:1 | 1 (-0.94268) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.14043 HOMO: -6.58788 LUMO: -0.78097 factor:1 | 1 (-0.25622) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.80535 HOMO: -6.67767 LUMO: -0.48436 factor:1 | -1 (0.07886) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.70413 HOMO: -6.63141 LUMO: -0.40545 factor:1 | -1 (1.18008) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.90834 HOMO: -6.62053 LUMO: -0.83811 factor:1 | 1 (-0.02414) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.22364 HOMO: -6.59604 LUMO: -0.35375 factor:1 | 1 (-0.33943) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.76828 HOMO: -6.34297 LUMO: -0.39729 factor:1 | -1 (2.11593) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.34349 HOMO: -6.67223 LUMO: 1.97827 factor:1 | -1 (0.54072) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.94209 HOMO: -6.40012 LUMO: 1.89935 factor:1 | 1 (-0.05788) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.09998 HOMO: -6.74842 LUMO: 1.97283 factor:1 | -1 (0.78423) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.76236 HOMO: -6.76747 LUMO: 2.17147 factor:1 | -1 (1.12184) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.63512 HOMO: -6.72121 LUMO: 1.55649 factor:1 | -1 (0.24909) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69259 HOMO: -6.97700 LUMO: 2.04085 factor:1 | -1 (0.19162) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.58951 HOMO: -7.06680 LUMO: 2.04085 factor:1 | -1 (0.29470) | 1 | 1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.49040 HOMO: -7.09673 LUMO: 2.35106 factor:1 | -1 (0.39380) | 1 | 1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.90218 HOMO: -6.83006 LUMO: 2.14970 factor:1 | -1 (0.98203) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.85215 HOMO: -6.72665 LUMO: 2.20140 factor:1 | -1 (0.03206) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.20697 HOMO: -6.77291 LUMO: 2.34562 factor:1 | -1 (0.67724) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.07647 HOMO: -6.73754 LUMO: 2.00276 factor:1 | -1 (0.80774) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62143 HOMO: -7.04231 LUMO: 1.92112 factor:1 | -1 (0.26278) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.74631 HOMO: -6.83822 LUMO: 1.72248 factor:1 | -1 (1.13790) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.01597 HOMO: -6.57971 LUMO: 2.16603 factor:1 | 1 (-0.13176) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.95011 HOMO: -6.80013 LUMO: 1.88575 factor:1 | 1 (-0.06591) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.76018 HOMO: -6.93618 LUMO: 2.18235 factor:1 | -1 (0.12403) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.89576 HOMO: -6.54706 LUMO: 1.91024 factor:1 | -1 (1.98844) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.60935 HOMO: -7.06952 LUMO: 2.18507 factor:1 | -1 (0.27486) | 1 | 1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96617 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-0.08196) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.09541 HOMO: -6.87632 LUMO: 1.92657 factor:1 | -1 (1.78879) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.08568 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-0.20147) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.67724 HOMO: -7.17292 LUMO: 1.90752 factor:1 | -1 (0.20697) | 1 | 1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.58516 HOMO: -6.93890 LUMO: 1.80684 factor:1 | -1 (1.29904) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.33628 HOMO: -7.10761 LUMO: 2.20956 factor:1 | -1 (0.54793) | 1 | 1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.51972 HOMO: -6.85727 LUMO: 2.13609 factor:1 | -1 (1.36449) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.53351 HOMO: -6.64502 LUMO: 1.38506 factor:1 | -1 (0.35070) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.45198 HOMO: -6.87360 LUMO: 1.15648 factor:1 | -1 (0.43223) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.37565 HOMO: -6.67223 LUMO: 2.07351 factor:1 | -1 (0.50855) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.90829 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-0.02408) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.67283 HOMO: -6.90897 LUMO: 2.28848 factor:1 | -1 (0.21138) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.96062 HOMO: -7.04231 LUMO: 1.70071 factor:1 | 1 (-0.07641) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.75634 HOMO: -6.69944 LUMO: 1.94834 factor:1 | -1 (0.12787) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.98609 HOMO: -6.56067 LUMO: 2.20956 factor:1 | 1 (-0.10188) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.78306 HOMO: -6.65046 LUMO: 2.06807 factor:1 | -1 (0.10114) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.74805 HOMO: -7.08584 LUMO: 1.98915 factor:1 | -1 (1.13616) | 1 | 1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.53781 HOMO: -6.69400 LUMO: 2.09256 factor:1 | -1 (0.34640) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.55896 HOMO: -6.62869 LUMO: 2.16331 factor:1 | -1 (1.32525) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.21162 HOMO: -6.85183 LUMO: 2.16058 factor:1 | -1 (0.67258) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.28574 HOMO: -6.54706 LUMO: 1.92384 factor:1 | -1 (2.59847) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.93187 HOMO: -6.84366 LUMO: 2.48984 factor:1 | -1 (1.95234) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12957.64926 HOMO: -6.77291 LUMO: 2.46263 factor:1 | -1 (2.23495) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.77901 HOMO: -7.01782 LUMO: 2.31025 factor:1 | -1 (0.10520) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.57408 HOMO: -6.94707 LUMO: 2.29664 factor:1 | -1 (0.31013) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.82932 HOMO: -6.64230 LUMO: 1.97283 factor:1 | -1 (0.05489) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.92955 HOMO: -6.47359 LUMO: 2.20412 factor:1 | -1 (0.95466) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.78731 HOMO: -6.90625 LUMO: 1.92384 factor:1 | -1 (0.09690) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.69109 HOMO: -7.17020 LUMO: 2.06807 factor:1 | -1 (0.19312) | 1 | 1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.56336 HOMO: -6.65046 LUMO: 2.20956 factor:1 | -1 (0.32085) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.97395 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-0.08974) | 1 | 1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.89267 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.00846) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.95294 HOMO: -6.92802 LUMO: 1.99187 factor:1 | 1 (-0.06874) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.19138 HOMO: -6.69672 LUMO: 2.36739 factor:1 | -1 (0.69283) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.25718 HOMO: -7.13755 LUMO: 2.00276 factor:1 | -1 (1.62702) | 1 | 1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.36872 HOMO: -6.92530 LUMO: 2.25582 factor:1 | -1 (0.51549) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12958.50075 HOMO: -6.77564 LUMO: 1.97827 factor:1 | -1 (1.38345) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.46605 HOMO: -6.87904 LUMO: 1.60003 factor:1 | -1 (0.41816) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.27861 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-0.39440) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.33692 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-0.45272) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.62004 HOMO: -6.74298 LUMO: 1.47486 factor:1 | -1 (0.26417) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12960.61992 HOMO: -6.77019 LUMO: 1.90480 factor:1 | 1 (-0.73571) | -1 | -1 |
| G: -6695.51851 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12959.92252 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-0.03831) | -1 | -1 |