乙二醇作为反应物的反应表19-17

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: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00227 HOMO: -6.91169 LUMO: -0.53879 factor:1 | 1 (-1.42827) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47753 HOMO: -7.29809 LUMO: 2.83543 factor:1 | -1 (0.09646) | 1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63803 HOMO: -6.86543 LUMO: -0.70205 factor:1 | 1 (-0.06403) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67141 HOMO: -7.47769 LUMO: 0.31293 factor:1 | 1 (-1.09741) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94814 HOMO: -6.63141 LUMO: -0.55511 factor:1 | -1 (0.62586) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.79932 HOMO: -6.68856 LUMO: -0.30205 factor:1 | -1 (0.77468) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89148 HOMO: -7.22190 LUMO: 0.53334 factor:1 | -1 (0.68252) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.57534 HOMO: -6.66407 LUMO: -0.27756 factor:1 | -1 (0.99866) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.75793 HOMO: -7.15659 LUMO: -0.70205 factor:1 | -1 (0.81607) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.56876 HOMO: -6.69400 LUMO: 1.67622 factor:1 | -1 (1.00524) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.36837 HOMO: -6.60420 LUMO: 2.16058 factor:1 | -1 (1.20563) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43824 HOMO: -6.87087 LUMO: 1.88031 factor:1 | -1 (0.13576) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94746 HOMO: -6.60965 LUMO: -0.19864 factor:1 | -1 (0.62654) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45226 HOMO: -7.29265 LUMO: 0.52246 factor:1 | -1 (0.12174) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75836 HOMO: -6.86543 LUMO: -0.59593 factor:1 | 1 (-0.18436) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.39187 HOMO: -7.44504 LUMO: -1.01226 factor:1 | -1 (0.18213) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64823 HOMO: -6.92530 LUMO: -0.75103 factor:1 | 1 (-0.07423) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70399 HOMO: -7.10489 LUMO: 2.20412 factor:1 | 1 (-0.12999) | 1 | 1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44621 HOMO: -6.58788 LUMO: 1.73881 factor:1 | 1 (-0.87221) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49657 HOMO: -6.64502 LUMO: 1.70343 factor:1 | 1 (-0.92257) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89105 HOMO: -6.73754 LUMO: 1.60819 factor:1 | -1 (0.68295) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97605 HOMO: -6.80829 LUMO: 2.45991 factor:1 | 1 (-0.40205) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19859 HOMO: -6.91713 LUMO: 2.43814 factor:1 | -1 (0.37541) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87719 HOMO: -6.60692 LUMO: 1.93745 factor:1 | 1 (-0.30319) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.80639 HOMO: -6.26134 LUMO: 1.46125 factor:1 | -1 (0.76761) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54758 HOMO: -7.54028 LUMO: 0.25851 factor:1 | -1 (0.02642) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53220 HOMO: -6.97700 LUMO: -0.73471 factor:1 | -1 (0.04180) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83210 HOMO: -6.92258 LUMO: -0.70205 factor:1 | 1 (-0.25810) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.48650 HOMO: -6.83550 LUMO: -0.56872 factor:1 | -1 (1.08750) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.85649 HOMO: -6.72121 LUMO: 1.89663 factor:1 | -1 (0.71751) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.73303 HOMO: -6.73482 LUMO: 1.89935 factor:1 | -1 (0.84097) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15576 HOMO: -6.61781 LUMO: 1.86670 factor:1 | -1 (0.41824) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94373 HOMO: -7.01782 LUMO: 2.26399 factor:1 | -1 (0.63027) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.49338 HOMO: -7.23551 LUMO: 2.09800 factor:1 | -1 (1.08062) | 1 | 1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81053 HOMO: -7.13483 LUMO: 2.17963 factor:1 | -1 (0.76347) | 1 | 1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.54941 HOMO: -6.22869 LUMO: 2.01092 factor:1 | -1 (1.02459) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.11464 HOMO: -6.80285 LUMO: 2.14970 factor:1 | -1 (0.45936) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94019 HOMO: -7.21102 LUMO: 2.33746 factor:1 | -1 (0.63381) | 1 | 1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74312 HOMO: -6.39740 LUMO: 2.59597 factor:1 | 1 (-0.16912) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55256 HOMO: -7.07768 LUMO: 2.48168 factor:1 | -1 (0.02144) | 1 | 1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.92865 HOMO: -7.11306 LUMO: 0.90614 factor:1 | -1 (0.64535) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.32773 HOMO: -6.61781 LUMO: -2.46263 factor:1 | 1 (-0.75373) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79693 HOMO: -6.96611 LUMO: 0.90614 factor:1 | 1 (-1.22293) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39845 HOMO: -6.86271 LUMO: -1.14832 factor:1 | 1 (-0.82445) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65610 HOMO: -6.72665 LUMO: 0.96873 factor:1 | 1 (-0.08210) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.23423 HOMO: -7.14571 LUMO: 1.05036 factor:1 | 1 (-0.66023) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44944 HOMO: -7.14299 LUMO: 0.98777 factor:1 | 1 (-0.87544) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78686 HOMO: -6.99333 LUMO: 1.05852 factor:1 | 1 (-1.21287) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76292 HOMO: -6.78924 LUMO: -1.49935 factor:1 | 1 (-1.18892) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.59559 HOMO: -7.13755 LUMO: 0.94151 factor:1 | 1 (-2.02159) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.64898 HOMO: -6.72938 LUMO: -0.35375 factor:1 | 1 (-2.07498) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.24129 HOMO: -6.99061 LUMO: 0.82450 factor:1 | 1 (-1.66730) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.98838 HOMO: -6.75114 LUMO: -0.68028 factor:1 | -1 (0.58562) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60521 HOMO: -6.40556 LUMO: -0.42722 factor:1 | 1 (-0.03121) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.73651 HOMO: -7.18653 LUMO: 0.42178 factor:1 | -1 (0.83748) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.53678 HOMO: -6.63958 LUMO: -0.71294 factor:1 | -1 (1.03722) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56698 HOMO: -6.63958 LUMO: -0.71022 factor:1 | -1 (0.00702) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38216 HOMO: -6.69672 LUMO: -0.72654 factor:1 | -1 (0.19184) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36550 HOMO: -6.56883 LUMO: -0.80274 factor:1 | 1 (-0.79150) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89282 HOMO: -6.68584 LUMO: -0.56872 factor:1 | -1 (0.68118) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43294 HOMO: -6.59060 LUMO: -0.35647 factor:1 | -1 (0.14106) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51245 HOMO: -6.72121 LUMO: -0.71838 factor:1 | -1 (0.06155) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.25323 HOMO: -6.57971 LUMO: -0.61498 factor:1 | -1 (0.32077) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.21568 HOMO: -7.07496 LUMO: 0.50613 factor:1 | -1 (0.35832) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50422 HOMO: -7.14027 LUMO: 0.43266 factor:1 | 1 (-0.93022) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47298 HOMO: -6.43277 LUMO: -0.44082 factor:1 | 1 (-0.89898) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28422 HOMO: -6.79468 LUMO: 0.07619 factor:1 | 1 (-0.71022) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83625 HOMO: -6.81917 LUMO: -2.57148 factor:1 | 1 (-1.26225) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79416 HOMO: -6.71849 LUMO: 1.30615 factor:1 | 1 (-1.22016) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84904 HOMO: -6.85455 LUMO: -0.63675 factor:1 | 1 (-1.27504) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.68704 HOMO: -6.73210 LUMO: -1.03131 factor:1 | 1 (-2.11305) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.65586 HOMO: -6.83550 LUMO: -0.58777 factor:1 | 1 (-2.08186) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73579 HOMO: -6.53073 LUMO: -0.74287 factor:1 | 1 (-1.16179) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.56936 HOMO: -7.18381 LUMO: -0.92791 factor:1 | 1 (-1.99536) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.42191 HOMO: -6.49264 LUMO: -0.44627 factor:1 | -1 (0.15208) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.40175 HOMO: -7.32803 LUMO: 0.41361 factor:1 | -1 (0.17225) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.27447 HOMO: -6.53073 LUMO: -0.52790 factor:1 | 1 (-1.70047) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.14308 HOMO: -6.54978 LUMO: -0.53062 factor:1 | -1 (0.43092) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.46069 HOMO: -6.56611 LUMO: -0.37824 factor:1 | -1 (0.11331) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51786 HOMO: -6.57155 LUMO: -0.64219 factor:1 | -1 (0.05614) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.14961 HOMO: -7.08040 LUMO: 0.45715 factor:1 | -1 (0.42439) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11458 HOMO: -6.66679 LUMO: -0.75376 factor:1 | 1 (-0.54058) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39023 HOMO: -6.83550 LUMO: -0.99322 factor:1 | 1 (-0.81623) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31711 HOMO: -6.53345 LUMO: -0.29660 factor:1 | 1 (-0.74312) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84232 HOMO: -6.65046 LUMO: 2.40549 factor:1 | 1 (-1.26832) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.67926 HOMO: -6.98788 LUMO: 2.01092 factor:1 | 1 (-2.10526) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.20896 HOMO: -6.61781 LUMO: 1.92384 factor:1 | -1 (0.36504) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77870 HOMO: -6.61237 LUMO: 2.06807 factor:1 | 1 (-1.20470) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.79064 HOMO: -6.59060 LUMO: 1.95106 factor:1 | 1 (-2.21664) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44131 HOMO: -6.48175 LUMO: 1.72248 factor:1 | 1 (-0.86731) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60210 HOMO: -6.84911 LUMO: 2.03541 factor:1 | 1 (-1.02810) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61317 HOMO: -6.50624 LUMO: 2.17147 factor:1 | 1 (-1.03918) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72349 HOMO: -6.68312 LUMO: 2.08439 factor:1 | 1 (-1.14949) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96938 HOMO: -6.96067 LUMO: 1.98099 factor:1 | 1 (-0.39538) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74202 HOMO: -6.93618 LUMO: 1.85854 factor:1 | 1 (-1.16802) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.15582 HOMO: -6.71305 LUMO: -0.61226 factor:1 | 1 (-1.58183) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39905 HOMO: -7.06408 LUMO: 0.80001 factor:1 | 1 (-0.82505) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94527 HOMO: -6.52257 LUMO: 0.99049 factor:1 | 1 (-0.37127) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66605 HOMO: -6.84638 LUMO: 1.10750 factor:1 | 1 (-1.09205) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86146 HOMO: -6.85455 LUMO: 0.84900 factor:1 | 1 (-0.28746) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71240 HOMO: -6.60148 LUMO: -0.78369 factor:1 | 1 (-0.13840) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73636 HOMO: -6.86543 LUMO: -0.93063 factor:1 | 1 (-1.16236) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06486 HOMO: -6.70489 LUMO: -0.72382 factor:1 | 1 (-1.49086) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62132 HOMO: -6.59060 LUMO: 0.31293 factor:1 | 1 (-0.04732) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48695 HOMO: -6.52257 LUMO: -0.48708 factor:1 | -1 (0.08705) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.37484 HOMO: -6.54706 LUMO: -0.48164 factor:1 | -1 (0.19916) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.23164 HOMO: -7.32803 LUMO: 0.08436 factor:1 | 1 (-0.65764) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62237 HOMO: -6.77291 LUMO: -0.66940 factor:1 | 1 (-1.04837) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.58405 HOMO: -6.68312 LUMO: -0.53062 factor:1 | -1 (0.98995) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.76672 HOMO: -7.07768 LUMO: 0.45987 factor:1 | -1 (0.80728) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.77404 HOMO: -6.50352 LUMO: -0.63675 factor:1 | -1 (0.79996) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56075 HOMO: -6.48992 LUMO: -0.60681 factor:1 | -1 (0.01325) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15301 HOMO: -6.65318 LUMO: -0.72382 factor:1 | -1 (0.42099) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71408 HOMO: -6.54706 LUMO: 0.24218 factor:1 | 1 (-0.14008) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55255 HOMO: -6.63958 LUMO: 0.57416 factor:1 | 1 (-0.97855) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77193 HOMO: -6.37563 LUMO: -0.48164 factor:1 | 1 (-0.19794) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79566 HOMO: -6.64774 LUMO: -0.71838 factor:1 | 1 (-0.22166) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61377 HOMO: -7.17020 LUMO: 0.45987 factor:1 | 1 (-1.03977) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13810 HOMO: -6.86543 LUMO: -1.05036 factor:1 | -1 (0.43590) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01575 HOMO: -6.77019 LUMO: -1.03131 factor:1 | 1 (-0.44175) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56447 HOMO: -6.80285 LUMO: 1.05852 factor:1 | -1 (0.00952) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48627 HOMO: -6.76475 LUMO: 1.01771 factor:1 | -1 (0.08773) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.37780 HOMO: -6.92530 LUMO: 1.37417 factor:1 | -1 (0.19619) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64736 HOMO: -6.98244 LUMO: 1.25989 factor:1 | 1 (-0.07336) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35595 HOMO: -6.74842 LUMO: 0.89798 factor:1 | 1 (-0.78195) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24539 HOMO: -6.77019 LUMO: -1.17009 factor:1 | 1 (-0.67139) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.83513 HOMO: -6.78652 LUMO: 1.35785 factor:1 | -1 (0.73887) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.79638 HOMO: -6.82734 LUMO: -0.68301 factor:1 | -1 (0.77762) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.80223 HOMO: -6.48175 LUMO: -2.19052 factor:1 | -1 (0.77177) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66668 HOMO: -6.65863 LUMO: -0.77008 factor:1 | 1 (-0.09268) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84929 HOMO: -6.44094 LUMO: -2.20956 factor:1 | 1 (-1.27529) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.88284 HOMO: -6.59876 LUMO: -0.57688 factor:1 | 1 (-1.30884) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89805 HOMO: -6.78380 LUMO: -0.77008 factor:1 | 1 (-1.32405) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.42211 HOMO: -7.30354 LUMO: 0.25034 factor:1 | 1 (-1.84812) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.03159 HOMO: -6.59332 LUMO: -0.53334 factor:1 | -1 (0.54240) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35511 HOMO: -6.64230 LUMO: -0.55783 factor:1 | -1 (0.21889) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84478 HOMO: -7.26544 LUMO: 0.20409 factor:1 | 1 (-0.27078) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10715 HOMO: -6.61237 LUMO: -0.65307 factor:1 | 1 (-0.53315) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.27184 HOMO: -6.72393 LUMO: -0.65307 factor:1 | -1 (0.30216) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.36042 HOMO: -6.29671 LUMO: -0.39729 factor:1 | -1 (0.21358) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.25519 HOMO: -6.75387 LUMO: -0.53334 factor:1 | -1 (0.31881) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.23322 HOMO: -6.53073 LUMO: -0.31293 factor:1 | 1 (-0.65922) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36373 HOMO: -6.42189 LUMO: -0.59049 factor:1 | 1 (-0.78973) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86690 HOMO: -6.41100 LUMO: -0.29933 factor:1 | 1 (-0.29290) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54136 HOMO: -6.57427 LUMO: -0.53879 factor:1 | 1 (-0.96736) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60396 HOMO: -7.43143 LUMO: 0.33470 factor:1 | 1 (-0.02996) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68926 HOMO: -6.56067 LUMO: -0.50885 factor:1 | 1 (-1.11526) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.71529 HOMO: -6.65863 LUMO: -0.76464 factor:1 | -1 (0.85871) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.59491 HOMO: -6.32665 LUMO: -0.41906 factor:1 | -1 (0.97909) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.74239 HOMO: -6.57699 LUMO: 1.63813 factor:1 | -1 (0.83161) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.48546 HOMO: -6.53073 LUMO: 1.71704 factor:1 | -1 (1.08854) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59482 HOMO: -6.86271 LUMO: 2.07351 factor:1 | 1 (-0.02082) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44915 HOMO: -6.63686 LUMO: 1.78235 factor:1 | -1 (0.12485) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.66971 HOMO: -6.60965 LUMO: 1.94289 factor:1 | -1 (0.90429) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.73572 HOMO: -6.55250 LUMO: 1.89119 factor:1 | -1 (0.83827) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.78936 HOMO: -6.50624 LUMO: 1.85582 factor:1 | -1 (0.78464) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.47175 HOMO: -6.06814 LUMO: 1.94561 factor:1 | -1 (1.10225) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60712 HOMO: -6.58788 LUMO: 2.01908 factor:1 | 1 (-0.03312) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.87907 HOMO: -6.74026 LUMO: 0.31293 factor:1 | -1 (0.69492) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67542 HOMO: -6.54434 LUMO: -0.42994 factor:1 | 1 (-0.10142) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53426 HOMO: -6.94707 LUMO: 0.42994 factor:1 | 1 (-0.96026) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.42806 HOMO: -6.98516 LUMO: 0.41361 factor:1 | -1 (0.14593) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75183 HOMO: -6.31304 LUMO: -0.54967 factor:1 | 1 (-0.17783) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.96169 HOMO: -6.48447 LUMO: -0.40817 factor:1 | -1 (0.61231) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.63583 HOMO: -6.49264 LUMO: 0.29116 factor:1 | -1 (0.93817) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81561 HOMO: -6.48719 LUMO: -0.11973 factor:1 | 1 (-0.24161) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50839 HOMO: -7.16204 LUMO: 0.44082 factor:1 | -1 (0.06561) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19282 HOMO: -6.74842 LUMO: -0.37552 factor:1 | -1 (0.38118) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.40333 HOMO: -6.44638 LUMO: -0.45171 factor:1 | -1 (0.17067) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13591 HOMO: -7.07496 LUMO: 0.50341 factor:1 | 1 (-0.56192) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51990 HOMO: -6.79468 LUMO: 0.11429 factor:1 | -1 (0.05410) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75302 HOMO: -6.63958 LUMO: -0.67484 factor:1 | 1 (-0.17902) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68374 HOMO: -7.08584 LUMO: 0.46259 factor:1 | 1 (-0.10974) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.39198 HOMO: -6.80285 LUMO: -0.73199 factor:1 | -1 (0.18202) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67875 HOMO: -6.44366 LUMO: -0.45443 factor:1 | 1 (-1.10476) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16612 HOMO: -6.75931 LUMO: 0.25851 factor:1 | 1 (-0.59212) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.73934 HOMO: -6.64502 LUMO: 1.79323 factor:1 | -1 (0.83465) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.79853 HOMO: -6.51168 LUMO: 1.60275 factor:1 | -1 (0.77547) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.74324 HOMO: -6.56067 LUMO: 1.63268 factor:1 | -1 (0.83076) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.52206 HOMO: -6.56883 LUMO: 1.70615 factor:1 | -1 (1.05194) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72105 HOMO: -6.77836 LUMO: 1.77962 factor:1 | 1 (-0.14705) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64312 HOMO: -6.38923 LUMO: 1.85854 factor:1 | 1 (-0.06912) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.22235 HOMO: -6.35658 LUMO: 2.16875 factor:1 | -1 (0.35165) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91166 HOMO: -6.83006 LUMO: 2.31025 factor:1 | 1 (-1.33766) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99462 HOMO: -6.87087 LUMO: 1.79051 factor:1 | 1 (-1.42062) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91443 HOMO: -6.56339 LUMO: 2.37828 factor:1 | 1 (-1.34043) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77892 HOMO: -6.30488 LUMO: 2.51705 factor:1 | 1 (-1.20492) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.78310 HOMO: -6.69400 LUMO: 1.95650 factor:1 | 1 (-2.20910) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.63651 HOMO: -6.51168 LUMO: 2.03541 factor:1 | 1 (-2.06251) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49203 HOMO: -6.30760 LUMO: 1.65173 factor:1 | 1 (-0.91803) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.75279 HOMO: -6.55250 LUMO: 1.90752 factor:1 | 1 (-2.17879) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.99282 HOMO: -6.41372 LUMO: 1.76058 factor:1 | -1 (0.58118) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.79333 HOMO: -6.23957 LUMO: 2.06534 factor:1 | -1 (0.78067) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.77975 HOMO: -6.58243 LUMO: 2.11705 factor:1 | -1 (0.79425) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80622 HOMO: -6.37835 LUMO: 2.09256 factor:1 | 1 (-0.23222) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68037 HOMO: -6.50624 LUMO: 2.55787 factor:1 | 1 (-0.10637) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52167 HOMO: -6.45454 LUMO: 1.87214 factor:1 | -1 (0.05233) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81550 HOMO: -6.53617 LUMO: 1.95650 factor:1 | 1 (-0.24150) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53655 HOMO: -6.51985 LUMO: 1.71432 factor:1 | 1 (-0.96255) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65724 HOMO: -6.75114 LUMO: 1.84493 factor:1 | 1 (-0.08324) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64224 HOMO: -6.06270 LUMO: 1.65717 factor:1 | 1 (-1.06824) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68614 HOMO: -5.89671 LUMO: 1.71704 factor:1 | 1 (-0.11214) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38551 HOMO: -6.18787 LUMO: 1.91840 factor:1 | -1 (0.18849) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75784 HOMO: -6.01644 LUMO: 1.85582 factor:1 | 1 (-0.18384) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55884 HOMO: -6.05998 LUMO: 2.33474 factor:1 | -1 (0.01516) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62956 HOMO: -6.05725 LUMO: 2.03541 factor:1 | 1 (-1.05556) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.25858 HOMO: -6.80829 LUMO: 1.90480 factor:1 | 1 (-0.68458) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24636 HOMO: -6.76475 LUMO: 2.20956 factor:1 | 1 (-0.67237) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14585 HOMO: -6.29944 LUMO: 1.77962 factor:1 | 1 (-0.57185) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70248 HOMO: -6.47359 LUMO: -0.25579 factor:1 | 1 (-1.12848) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59834 HOMO: -6.57699 LUMO: -0.47348 factor:1 | 1 (-1.02435) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93495 HOMO: -7.20830 LUMO: 0.49797 factor:1 | 1 (-1.36095) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80371 HOMO: -7.49402 LUMO: 0.29933 factor:1 | 1 (-1.22971) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.66174 HOMO: -6.66679 LUMO: -0.58777 factor:1 | 1 (-2.08774) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74428 HOMO: -6.67767 LUMO: -0.56328 factor:1 | 1 (-1.17028) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.61142 HOMO: -7.42871 LUMO: 0.35647 factor:1 | 1 (-2.03743) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.77701 HOMO: -6.56067 LUMO: -0.54423 factor:1 | 1 (-2.20301) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86380 HOMO: -6.56339 LUMO: -0.50341 factor:1 | 1 (-0.28980) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07779 HOMO: -6.56067 LUMO: -0.48436 factor:1 | 1 (-0.50379) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67786 HOMO: -6.73210 LUMO: 1.75241 factor:1 | 1 (-1.10386) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72885 HOMO: -6.48175 LUMO: 1.91296 factor:1 | 1 (-1.15485) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86289 HOMO: -6.67767 LUMO: 1.70343 factor:1 | 1 (-1.28889) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30250 HOMO: -6.37835 LUMO: 1.96466 factor:1 | 1 (-0.72850) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57046 HOMO: -6.40828 LUMO: 2.10072 factor:1 | -1 (0.00354) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15493 HOMO: -6.06542 LUMO: 1.92112 factor:1 | 1 (-0.58094) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00116 HOMO: -6.90353 LUMO: 1.83133 factor:1 | 1 (-0.42716) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12873 HOMO: -6.37019 LUMO: 1.92929 factor:1 | 1 (-0.55473) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30136 HOMO: -6.61509 LUMO: 2.11160 factor:1 | 1 (-0.72736) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.88012 HOMO: -6.82734 LUMO: 1.77146 factor:1 | 1 (-1.30612) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08886 HOMO: -6.01100 LUMO: 1.89935 factor:1 | 1 (-1.51486) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89479 HOMO: -6.49536 LUMO: 1.75241 factor:1 | 1 (-0.32080) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84470 HOMO: -6.34297 LUMO: 1.86398 factor:1 | 1 (-0.27070) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75985 HOMO: -6.53073 LUMO: 1.84493 factor:1 | 1 (-0.18585) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86428 HOMO: -6.53345 LUMO: 2.41093 factor:1 | 1 (-1.29028) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.92899 HOMO: -7.01237 LUMO: 2.06262 factor:1 | -1 (1.64501) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.74240 HOMO: -6.17154 LUMO: 1.89119 factor:1 | -1 (1.83160) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.87826 HOMO: -6.08719 LUMO: 1.74425 factor:1 | -1 (0.69574) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.25561 HOMO: -6.69672 LUMO: 1.95106 factor:1 | -1 (1.31839) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.55776 HOMO: -6.58243 LUMO: 2.24766 factor:1 | -1 (1.01624) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.46192 HOMO: -6.74570 LUMO: 2.02181 factor:1 | -1 (1.11207) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.79834 HOMO: -6.53890 LUMO: 1.92929 factor:1 | -1 (0.77566) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.43531 HOMO: -6.03276 LUMO: 1.67078 factor:1 | -1 (1.13869) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50649 HOMO: -6.67767 LUMO: 2.03541 factor:1 | -1 (0.06751) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35974 HOMO: -5.98378 LUMO: 1.84221 factor:1 | -1 (0.21426) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73806 HOMO: -6.07086 LUMO: 2.01908 factor:1 | 1 (-0.16406) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44768 HOMO: -6.29944 LUMO: 1.90208 factor:1 | -1 (0.12632) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85055 HOMO: -6.75114 LUMO: 1.85854 factor:1 | 1 (-0.27655) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93190 HOMO: -6.56611 LUMO: 2.49801 factor:1 | 1 (-1.35790) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73829 HOMO: -6.39740 LUMO: 1.92929 factor:1 | 1 (-1.16429) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.67086 HOMO: -6.85999 LUMO: -1.07757 factor:1 | -1 (1.90314) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.68254 HOMO: -6.98244 LUMO: 1.07213 factor:1 | -1 (1.89146) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.56198 HOMO: -7.04231 LUMO: 0.64219 factor:1 | -1 (1.01202) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.10137 HOMO: -6.96339 LUMO: 0.75648 factor:1 | -1 (1.47263) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.41093 HOMO: -6.83822 LUMO: -0.97417 factor:1 | -1 (1.16307) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.35082 HOMO: -6.44910 LUMO: -2.15242 factor:1 | -1 (1.22318) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.34545 HOMO: -6.84094 LUMO: -1.37690 factor:1 | -1 (0.22855) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41235 HOMO: -6.74026 LUMO: -2.54699 factor:1 | 1 (-0.83836) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15385 HOMO: -6.96611 LUMO: 1.24900 factor:1 | 1 (-0.57985) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98760 HOMO: -7.21102 LUMO: 0.82995 factor:1 | 1 (-1.41360) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87126 HOMO: -6.88448 LUMO: 0.81634 factor:1 | 1 (-0.29726) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00948 HOMO: -7.04231 LUMO: 1.10750 factor:1 | 1 (-1.43548) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76456 HOMO: -6.83550 LUMO: -0.98777 factor:1 | 1 (-0.19056) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06848 HOMO: -6.82189 LUMO: 0.93879 factor:1 | 1 (-0.49449) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78826 HOMO: -6.81101 LUMO: 0.70750 factor:1 | 1 (-0.21426) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50594 HOMO: -7.06680 LUMO: 0.74015 factor:1 | -1 (0.06806) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64441 HOMO: -6.68856 LUMO: 0.86260 factor:1 | 1 (-1.07041) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.68938 HOMO: -6.83822 LUMO: -0.63403 factor:1 | -1 (0.88461) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.48650 HOMO: -6.84911 LUMO: 1.26533 factor:1 | -1 (1.08750) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.43074 HOMO: -7.01237 LUMO: 0.73743 factor:1 | -1 (1.14326) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.44173 HOMO: -7.00965 LUMO: 1.40139 factor:1 | -1 (1.13227) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54714 HOMO: -6.73210 LUMO: -2.49256 factor:1 | -1 (0.02686) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43106 HOMO: -7.08040 LUMO: 0.84627 factor:1 | -1 (0.14294) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.22022 HOMO: -7.00965 LUMO: 0.82995 factor:1 | -1 (0.35378) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74624 HOMO: -6.88448 LUMO: 0.82723 factor:1 | 1 (-1.17224) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28220 HOMO: -7.20013 LUMO: 0.88437 factor:1 | 1 (-0.70820) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09044 HOMO: -6.60420 LUMO: -0.53334 factor:1 | 1 (-0.51644) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94962 HOMO: -6.78652 LUMO: -0.79729 factor:1 | 1 (-1.37562) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07398 HOMO: -6.48992 LUMO: -0.64491 factor:1 | 1 (-0.49998) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91427 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-1.34027) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98914 HOMO: -6.65046 LUMO: -0.78097 factor:1 | 1 (-0.41514) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06548 HOMO: -7.24095 LUMO: 0.37280 factor:1 | 1 (-1.49148) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84845 HOMO: -6.81101 LUMO: -0.74831 factor:1 | 1 (-0.27445) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70433 HOMO: -6.69400 LUMO: -0.77280 factor:1 | 1 (-1.13033) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79429 HOMO: -6.08447 LUMO: -0.68573 factor:1 | 1 (-1.22029) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12650 HOMO: -6.66679 LUMO: -0.47076 factor:1 | 1 (-0.55250) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57604 HOMO: -6.97428 LUMO: -1.10750 factor:1 | 1 (-0.00204) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.50954 HOMO: -6.69128 LUMO: -0.54151 factor:1 | -1 (1.06445) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28076 HOMO: -6.53617 LUMO: -0.35375 factor:1 | 1 (-0.70676) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48351 HOMO: -6.75659 LUMO: -0.41361 factor:1 | 1 (-0.90951) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43110 HOMO: -6.69400 LUMO: -0.67484 factor:1 | 1 (-0.85710) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44747 HOMO: -6.89264 LUMO: -0.90886 factor:1 | -1 (0.12653) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23166 HOMO: -6.56339 LUMO: -0.52518 factor:1 | 1 (-1.65766) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.46708 HOMO: -6.45726 LUMO: -0.65852 factor:1 | 1 (-0.89308) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49222 HOMO: -6.80557 LUMO: -0.56600 factor:1 | 1 (-0.91822) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89190 HOMO: -7.19469 LUMO: -0.91702 factor:1 | 1 (-1.31790) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51829 HOMO: -6.41100 LUMO: 0.79185 factor:1 | 1 (-0.94429) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42457 HOMO: -6.39195 LUMO: 0.26123 factor:1 | 1 (-0.85057) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12791 HOMO: -6.78924 LUMO: 0.35919 factor:1 | 1 (-0.55391) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.17201 HOMO: -6.50624 LUMO: 0.71838 factor:1 | -1 (0.40199) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50438 HOMO: -6.68584 LUMO: -0.66124 factor:1 | 1 (-0.93038) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.58466 HOMO: -6.45182 LUMO: -0.48980 factor:1 | 1 (-1.01066) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89204 HOMO: -7.18925 LUMO: -1.01498 factor:1 | 1 (-1.31804) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20889 HOMO: -7.18925 LUMO: -0.63130 factor:1 | 1 (-0.63490) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87528 HOMO: -6.66679 LUMO: -0.57960 factor:1 | 1 (-0.30128) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13034 HOMO: -6.44910 LUMO: -0.30205 factor:1 | 1 (-0.55634) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29725 HOMO: -7.23279 LUMO: 0.46804 factor:1 | 1 (-0.72325) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33273 HOMO: -6.92802 LUMO: -0.72927 factor:1 | 1 (-0.75874) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23134 HOMO: -6.83278 LUMO: -0.59321 factor:1 | 1 (-1.65734) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99084 HOMO: -7.44776 LUMO: 0.27211 factor:1 | 1 (-1.41684) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.22423 HOMO: -6.80829 LUMO: -0.59865 factor:1 | 1 (-1.65023) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13050 HOMO: -6.63686 LUMO: -0.75103 factor:1 | 1 (-0.55650) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16040 HOMO: -6.73210 LUMO: -0.55511 factor:1 | 1 (-0.58641) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86122 HOMO: -6.50624 LUMO: 1.58642 factor:1 | 1 (-0.28722) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.11395 HOMO: -6.79196 LUMO: 0.96328 factor:1 | 1 (-1.53995) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.14091 HOMO: -6.82734 LUMO: 1.23540 factor:1 | 1 (-1.56691) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.10910 HOMO: -6.90081 LUMO: 1.25444 factor:1 | 1 (-1.53510) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22672 HOMO: -7.00965 LUMO: -1.05036 factor:1 | 1 (-0.65272) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.32922 HOMO: -7.01237 LUMO: -1.48302 factor:1 | 1 (-0.75522) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93643 HOMO: -6.91713 LUMO: 0.93607 factor:1 | 1 (-0.36243) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67196 HOMO: -7.02598 LUMO: 0.92247 factor:1 | 1 (-0.09796) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.05068 HOMO: -6.98516 LUMO: 1.52384 factor:1 | 1 (-1.47668) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.88752 HOMO: -6.75387 LUMO: 1.04764 factor:1 | 1 (-1.31352) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.32894 HOMO: -7.09401 LUMO: 1.19458 factor:1 | -1 (1.24506) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.09726 HOMO: -6.88992 LUMO: -1.56193 factor:1 | -1 (0.47674) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.95448 HOMO: -7.00149 LUMO: 0.99866 factor:1 | -1 (0.61952) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.84199 HOMO: -7.13755 LUMO: 1.05308 factor:1 | -1 (1.73200) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.37070 HOMO: -6.85183 LUMO: -1.42860 factor:1 | -1 (0.20330) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.28915 HOMO: -6.63141 LUMO: -0.88981 factor:1 | -1 (0.28485) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.20042 HOMO: -6.92258 LUMO: -0.82178 factor:1 | -1 (1.37358) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74241 HOMO: -6.55794 LUMO: -0.80818 factor:1 | 1 (-0.16841) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96133 HOMO: -6.95251 LUMO: -0.97145 factor:1 | 1 (-0.38733) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.17401 HOMO: -7.37701 LUMO: 0.14150 factor:1 | 1 (-0.60001) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83114 HOMO: -6.74842 LUMO: -0.68028 factor:1 | 1 (-1.25714) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.36998 HOMO: -6.65046 LUMO: -0.52518 factor:1 | 1 (-1.79598) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.36415 HOMO: -6.91441 LUMO: -1.13199 factor:1 | 1 (-1.79016) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.56417 HOMO: -7.00965 LUMO: -1.00682 factor:1 | 1 (-0.99017) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19711 HOMO: -6.55794 LUMO: -0.54967 factor:1 | 1 (-0.62311) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.10464 HOMO: -6.71577 LUMO: -0.53879 factor:1 | 1 (-1.53064) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.21894 HOMO: -6.88992 LUMO: -0.55511 factor:1 | -1 (0.35505) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.04879 HOMO: -6.74026 LUMO: -0.60681 factor:1 | -1 (0.52521) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89090 HOMO: -6.76747 LUMO: -0.50885 factor:1 | 1 (-0.31690) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99281 HOMO: -6.87904 LUMO: -0.92519 factor:1 | 1 (-0.41881) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94416 HOMO: -6.53073 LUMO: -0.53062 factor:1 | 1 (-0.37016) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09110 HOMO: -6.97700 LUMO: -0.98505 factor:1 | 1 (-0.51710) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09853 HOMO: -6.96884 LUMO: -0.79185 factor:1 | 1 (-0.52453) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.16029 HOMO: -6.60420 LUMO: -0.31021 factor:1 | 1 (-1.58629) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.37713 HOMO: -6.68584 LUMO: -0.63947 factor:1 | 1 (-1.80314) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.29270 HOMO: -6.41917 LUMO: -0.35103 factor:1 | 1 (-1.71870) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.36130 HOMO: -6.73482 LUMO: -0.70477 factor:1 | 1 (-1.78730) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67614 HOMO: -6.71305 LUMO: -0.85716 factor:1 | 1 (-1.10214) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47377 HOMO: -6.70761 LUMO: -0.63403 factor:1 | 1 (-0.89977) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.47237 HOMO: -6.37563 LUMO: -0.38640 factor:1 | 1 (-1.89838) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.11547 HOMO: -6.27495 LUMO: -0.54967 factor:1 | 1 (-1.54147) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23819 HOMO: -6.98516 LUMO: 0.38096 factor:1 | 1 (-1.66419) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.25150 HOMO: -6.47087 LUMO: -0.40001 factor:1 | 1 (-1.67750) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.34902 HOMO: -6.59876 LUMO: 0.20681 factor:1 | 1 (-1.77503) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.28603 HOMO: -6.89809 LUMO: 0.14966 factor:1 | 1 (-1.71203) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.31085 HOMO: -6.76203 LUMO: 2.11432 factor:1 | 1 (-1.73685) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31807 HOMO: -6.58516 LUMO: 1.75786 factor:1 | 1 (-0.74407) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.03682 HOMO: -6.37835 LUMO: 1.84493 factor:1 | -1 (0.53718) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.09905 HOMO: -6.83550 LUMO: 1.74425 factor:1 | -1 (0.47495) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93735 HOMO: -6.65318 LUMO: 1.79051 factor:1 | 1 (-0.36335) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07368 HOMO: -6.68584 LUMO: 2.11160 factor:1 | 1 (-0.49968) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06783 HOMO: -6.36202 LUMO: 1.85037 factor:1 | 1 (-0.49383) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00652 HOMO: -6.68312 LUMO: 2.23133 factor:1 | 1 (-1.43252) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16315 HOMO: -6.66679 LUMO: 2.14154 factor:1 | 1 (-0.58915) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19657 HOMO: -6.50896 LUMO: 1.92657 factor:1 | 1 (-0.62257) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92918 HOMO: -6.63686 LUMO: 2.22317 factor:1 | 1 (-1.35518) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05390 HOMO: -6.58788 LUMO: 2.17419 factor:1 | 1 (-0.47990) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.03003 HOMO: -6.72665 LUMO: 2.12249 factor:1 | 1 (-1.45603) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.50764 HOMO: -6.28311 LUMO: 1.91024 factor:1 | -1 (1.06636) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45239 HOMO: -6.56067 LUMO: 2.27487 factor:1 | -1 (0.12161) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68178 HOMO: -6.83006 LUMO: 2.28031 factor:1 | 1 (-0.10778) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.41772 HOMO: -6.45182 LUMO: 1.62724 factor:1 | -1 (0.15627) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43192 HOMO: -6.78380 LUMO: 1.83677 factor:1 | 1 (-0.85792) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28204 HOMO: -6.23413 LUMO: 1.80956 factor:1 | 1 (-0.70804) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53785 HOMO: -6.74298 LUMO: 2.16875 factor:1 | 1 (-0.96385) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45642 HOMO: -6.81645 LUMO: 2.50073 factor:1 | -1 (0.11758) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.72903 HOMO: -6.71033 LUMO: 1.96466 factor:1 | -1 (0.84497) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47712 HOMO: -6.83550 LUMO: 2.04358 factor:1 | 1 (-0.90312) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.72949 HOMO: -6.60965 LUMO: 2.38100 factor:1 | -1 (0.84451) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19266 HOMO: -6.73210 LUMO: 2.26127 factor:1 | -1 (0.38134) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.56726 HOMO: -6.76203 LUMO: 2.13609 factor:1 | -1 (1.00674) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05746 HOMO: -6.71033 LUMO: 2.05990 factor:1 | 1 (-0.48346) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.17085 HOMO: -6.50896 LUMO: 2.32385 factor:1 | 1 (-0.59685) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09893 HOMO: -6.53345 LUMO: 1.74425 factor:1 | 1 (-0.52493) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36599 HOMO: -6.25862 LUMO: 1.63540 factor:1 | 1 (-0.79199) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29652 HOMO: -5.90759 LUMO: 1.78779 factor:1 | 1 (-0.72252) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30416 HOMO: -6.09807 LUMO: 1.99732 factor:1 | 1 (-0.73016) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04416 HOMO: -5.92392 LUMO: 1.99732 factor:1 | 1 (-0.47016) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85345 HOMO: -6.45182 LUMO: 1.72248 factor:1 | 1 (-1.27945) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77906 HOMO: -6.53073 LUMO: 1.82588 factor:1 | 1 (-1.20506) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68275 HOMO: -6.40828 LUMO: 2.05174 factor:1 | 1 (-1.10876) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.12045 HOMO: -6.60420 LUMO: -0.82450 factor:1 | 1 (-1.54645) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87693 HOMO: -6.76747 LUMO: -0.57144 factor:1 | 1 (-1.30294) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50027 HOMO: -6.67767 LUMO: -0.59321 factor:1 | 1 (-0.92628) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.98316 HOMO: -6.65863 LUMO: -0.57416 factor:1 | -1 (0.59084) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13731 HOMO: -6.49808 LUMO: -0.54695 factor:1 | -1 (0.43669) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.14420 HOMO: -6.50080 LUMO: -0.61498 factor:1 | -1 (0.42980) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15515 HOMO: -6.74842 LUMO: -0.51974 factor:1 | 1 (-0.58115) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97191 HOMO: -6.13345 LUMO: 0.67756 factor:1 | 1 (-0.39791) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11937 HOMO: -6.48719 LUMO: 0.52790 factor:1 | 1 (-0.54537) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86225 HOMO: -6.35930 LUMO: 0.74015 factor:1 | 1 (-0.28825) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88271 HOMO: -6.41644 LUMO: 0.22313 factor:1 | 1 (-0.30871) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.19879 HOMO: -6.85727 LUMO: -0.00272 factor:1 | 1 (-1.62479) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61239 HOMO: -6.84638 LUMO: 0.24762 factor:1 | 1 (-0.03840) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.30717 HOMO: -6.66951 LUMO: 0.39184 factor:1 | 1 (-1.73317) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.05484 HOMO: -6.62597 LUMO: -0.65035 factor:1 | 1 (-1.48084) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.14630 HOMO: -7.13755 LUMO: 0.45715 factor:1 | 1 (-1.57230) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17558 HOMO: -7.12666 LUMO: 0.45171 factor:1 | 1 (-1.60158) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43152 HOMO: -6.46270 LUMO: -0.46259 factor:1 | -1 (0.14248) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.23097 HOMO: -6.36202 LUMO: -0.29660 factor:1 | -1 (0.34303) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.26921 HOMO: -6.28583 LUMO: 0.40545 factor:1 | -1 (1.30479) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45016 HOMO: -6.70761 LUMO: 0.41906 factor:1 | -1 (0.12384) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.36262 HOMO: -6.76203 LUMO: -0.60954 factor:1 | -1 (0.21138) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.05661 HOMO: -6.85999 LUMO: -0.75103 factor:1 | -1 (1.51739) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66176 HOMO: -7.19741 LUMO: -1.00954 factor:1 | 1 (-0.08776) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56622 HOMO: -6.58243 LUMO: -0.33470 factor:1 | -1 (0.00778) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21513 HOMO: -7.22190 LUMO: 0.49253 factor:1 | 1 (-0.64113) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33227 HOMO: -7.22462 LUMO: 0.51974 factor:1 | 1 (-0.75827) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.64571 HOMO: -7.08584 LUMO: -0.68301 factor:1 | -1 (0.92829) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94871 HOMO: -6.68584 LUMO: -0.29660 factor:1 | -1 (0.62529) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.25927 HOMO: -6.33753 LUMO: -0.48436 factor:1 | -1 (0.31473) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89849 HOMO: -7.15932 LUMO: 0.55511 factor:1 | 1 (-0.32450) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84524 HOMO: -6.57427 LUMO: 2.01908 factor:1 | 1 (-0.27124) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96010 HOMO: -6.75659 LUMO: 2.22045 factor:1 | 1 (-0.38610) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86505 HOMO: -6.73482 LUMO: 2.20956 factor:1 | 1 (-0.29105) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02990 HOMO: -6.74026 LUMO: 1.76602 factor:1 | 1 (-0.45590) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91806 HOMO: -6.95523 LUMO: 1.94834 factor:1 | 1 (-0.34406) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19279 HOMO: -6.33209 LUMO: 1.87486 factor:1 | 1 (-0.61879) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55225 HOMO: -6.71033 LUMO: 2.12521 factor:1 | 1 (-0.97825) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.58618 HOMO: -6.50080 LUMO: 2.04902 factor:1 | 1 (-1.01218) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65796 HOMO: -6.76475 LUMO: 1.94017 factor:1 | 1 (-1.08397) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77291 HOMO: -6.53073 LUMO: 2.08983 factor:1 | 1 (-1.19891) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20917 HOMO: -6.69944 LUMO: 2.20684 factor:1 | 1 (-0.63517) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85683 HOMO: -6.34570 LUMO: 1.80684 factor:1 | 1 (-1.28283) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80295 HOMO: -6.78380 LUMO: 1.95922 factor:1 | 1 (-1.22895) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06257 HOMO: -6.93618 LUMO: 1.76058 factor:1 | 1 (-1.48857) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31831 HOMO: -6.93346 LUMO: 1.79595 factor:1 | 1 (-0.74431) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.58275 HOMO: -6.29671 LUMO: 1.75241 factor:1 | 1 (-1.00875) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23278 HOMO: -6.77019 LUMO: 1.74697 factor:1 | 1 (-1.65878) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.08297 HOMO: -6.87360 LUMO: 1.91024 factor:1 | -1 (0.49103) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.36654 HOMO: -6.32665 LUMO: 1.87759 factor:1 | -1 (0.20746) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12097 HOMO: -6.99877 LUMO: 1.99187 factor:1 | 1 (-0.54698) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00318 HOMO: -6.72665 LUMO: 2.12521 factor:1 | 1 (-0.42918) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11627 HOMO: -6.67767 LUMO: 2.43814 factor:1 | 1 (-0.54227) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.20301 HOMO: -6.99605 LUMO: 1.79051 factor:1 | -1 (1.37099) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70033 HOMO: -6.25046 LUMO: 1.77146 factor:1 | 1 (-1.12633) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.40056 HOMO: -6.30488 LUMO: 1.90480 factor:1 | 1 (-1.82656) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77840 HOMO: -6.38379 LUMO: 1.68438 factor:1 | 1 (-1.20440) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36531 HOMO: -6.78924 LUMO: 2.01364 factor:1 | 1 (-0.79131) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.04226 HOMO: -6.15249 LUMO: 1.98643 factor:1 | -1 (0.53174) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.06985 HOMO: -6.19331 LUMO: 2.14154 factor:1 | -1 (0.50415) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38940 HOMO: -6.05998 LUMO: 2.12521 factor:1 | -1 (0.18460) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93324 HOMO: -6.67223 LUMO: 1.91840 factor:1 | 1 (-0.35924) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92745 HOMO: -6.79196 LUMO: 2.18507 factor:1 | 1 (-0.35345) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74333 HOMO: -6.93346 LUMO: 1.78235 factor:1 | 1 (-1.16933) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.11890 HOMO: -6.16882 LUMO: 1.80956 factor:1 | 1 (-1.54490) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05028 HOMO: -6.72665 LUMO: 2.07895 factor:1 | 1 (-0.47628) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86853 HOMO: -6.73210 LUMO: 1.97827 factor:1 | 1 (-0.29454) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07044 HOMO: -6.84638 LUMO: 1.87214 factor:1 | 1 (-0.49644) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.40169 HOMO: -6.83006 LUMO: 2.36195 factor:1 | 1 (-0.82769) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01805 HOMO: -6.97700 LUMO: 1.91024 factor:1 | 1 (-1.44405) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66249 HOMO: -6.20420 LUMO: 1.81772 factor:1 | 1 (-0.08849) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16492 HOMO: -7.09129 LUMO: 2.10344 factor:1 | 1 (-0.59092) | 1 | 1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09406 HOMO: -6.77564 LUMO: 2.14970 factor:1 | 1 (-0.52006) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05243 HOMO: -6.81645 LUMO: 1.85854 factor:1 | 1 (-0.47843) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03559 HOMO: -6.50896 LUMO: 2.04358 factor:1 | 1 (-0.46159) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89550 HOMO: -6.89264 LUMO: 1.66262 factor:1 | 1 (-0.32150) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83025 HOMO: -6.75931 LUMO: 2.23950 factor:1 | 1 (-0.25625) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11978 HOMO: -6.50080 LUMO: 1.67622 factor:1 | 1 (-0.54578) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14076 HOMO: -6.30216 LUMO: 2.24222 factor:1 | 1 (-0.56676) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05159 HOMO: -7.18108 LUMO: 2.10072 factor:1 | 1 (-0.47759) | 1 | 1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84470 HOMO: -6.54162 LUMO: 2.35378 factor:1 | 1 (-0.27070) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89959 HOMO: -5.98650 LUMO: 1.48302 factor:1 | -1 (0.67441) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88492 HOMO: -7.15115 LUMO: 2.14970 factor:1 | 1 (-0.31092) | 1 | 1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66069 HOMO: -6.45454 LUMO: 2.15786 factor:1 | 1 (-0.08670) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20615 HOMO: -7.06952 LUMO: 2.14970 factor:1 | 1 (-0.63215) | 1 | 1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06462 HOMO: -6.93618 LUMO: 1.86942 factor:1 | 1 (-0.49062) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08299 HOMO: -6.63141 LUMO: 1.92657 factor:1 | 1 (-0.50899) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31393 HOMO: -6.51441 LUMO: -0.44355 factor:1 | 1 (-0.73993) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38348 HOMO: -6.82734 LUMO: -1.03131 factor:1 | 1 (-0.80948) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42212 HOMO: -6.58788 LUMO: -0.82995 factor:1 | 1 (-0.84812) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.24199 HOMO: -6.43277 LUMO: -0.40817 factor:1 | -1 (0.33201) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.75143 HOMO: -6.78924 LUMO: -0.72110 factor:1 | -1 (0.82257) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41374 HOMO: -7.28177 LUMO: 0.36735 factor:1 | 1 (-0.83974) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62795 HOMO: -6.47903 LUMO: -0.46259 factor:1 | 1 (-1.05395) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69119 HOMO: -6.67495 LUMO: -0.75376 factor:1 | 1 (-1.11719) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82134 HOMO: -6.71033 LUMO: -0.71838 factor:1 | 1 (-1.24734) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72012 HOMO: -6.79740 LUMO: -0.79185 factor:1 | 1 (-1.14612) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91174 HOMO: -6.08719 LUMO: -0.63675 factor:1 | 1 (-1.33774) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.96525 HOMO: -6.84094 LUMO: 0.42994 factor:1 | -1 (0.60875) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.97241 HOMO: -6.59604 LUMO: 0.25851 factor:1 | -1 (0.60159) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77553 HOMO: -6.82462 LUMO: 0.08708 factor:1 | 1 (-0.20153) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99648 HOMO: -6.54706 LUMO: 0.44082 factor:1 | 1 (-0.42248) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90486 HOMO: -6.99333 LUMO: 0.32109 factor:1 | 1 (-0.33086) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86935 HOMO: -6.29944 LUMO: -0.57144 factor:1 | 1 (-0.29535) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94729 HOMO: -6.57699 LUMO: -0.46531 factor:1 | -1 (0.62671) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00187 HOMO: -6.24773 LUMO: -0.53879 factor:1 | 1 (-0.42787) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86824 HOMO: -6.96067 LUMO: -0.67212 factor:1 | 1 (-0.29424) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.64340 HOMO: -7.24095 LUMO: -0.09252 factor:1 | -1 (0.93060) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97801 HOMO: -6.33481 LUMO: -0.46531 factor:1 | 1 (-0.40401) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.30021 HOMO: -6.43549 LUMO: -0.33198 factor:1 | 1 (-1.72621) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.14978 HOMO: -6.53073 LUMO: 0.44899 factor:1 | 1 (-1.57578) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.31749 HOMO: -6.69128 LUMO: 0.47620 factor:1 | 1 (-1.74349) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.02038 HOMO: -6.65318 LUMO: 0.52246 factor:1 | 1 (-2.44639) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.97780 HOMO: -6.71305 LUMO: 0.41089 factor:1 | 1 (-2.40380) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.27838 HOMO: -6.70216 LUMO: 0.19864 factor:1 | 1 (-1.70439) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.78745 HOMO: -6.41100 LUMO: 0.34558 factor:1 | 1 (-2.21346) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.08858 HOMO: -7.01237 LUMO: 0.02993 factor:1 | 1 (-2.51458) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.41338 HOMO: -6.85999 LUMO: 0.18776 factor:1 | 1 (-1.83938) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.35218 HOMO: -6.62869 LUMO: 0.48708 factor:1 | 1 (-1.77818) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.32383 HOMO: -6.43821 LUMO: -0.45715 factor:1 | 1 (-1.74983) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.16724 HOMO: -6.43277 LUMO: -0.72110 factor:1 | -1 (0.40676) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13516 HOMO: -7.10761 LUMO: 0.43266 factor:1 | -1 (0.43884) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07651 HOMO: -6.57699 LUMO: -0.61498 factor:1 | 1 (-0.50251) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89678 HOMO: -6.82189 LUMO: -0.75648 factor:1 | 1 (-0.32278) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03368 HOMO: -6.55794 LUMO: -0.67212 factor:1 | 1 (-0.45968) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95918 HOMO: -6.69128 LUMO: 1.88575 factor:1 | 1 (-0.38518) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86320 HOMO: -6.65591 LUMO: 1.70888 factor:1 | 1 (-0.28920) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02582 HOMO: -6.58788 LUMO: 1.68438 factor:1 | 1 (-0.45182) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85078 HOMO: -6.46270 LUMO: 1.72520 factor:1 | 1 (-1.27679) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81759 HOMO: -6.57427 LUMO: 1.73881 factor:1 | 1 (-1.24359) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94913 HOMO: -6.45182 LUMO: 1.75241 factor:1 | 1 (-1.37513) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89888 HOMO: -6.51441 LUMO: 1.78779 factor:1 | 1 (-0.32488) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67476 HOMO: -6.67495 LUMO: 2.11705 factor:1 | 1 (-0.10076) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82129 HOMO: -6.22597 LUMO: 1.96466 factor:1 | 1 (-1.24729) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55162 HOMO: -6.68040 LUMO: 2.30753 factor:1 | 1 (-0.97762) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78292 HOMO: -6.65046 LUMO: 2.18235 factor:1 | 1 (-1.20892) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83538 HOMO: -6.38651 LUMO: 1.76874 factor:1 | 1 (-1.26138) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42514 HOMO: -6.41644 LUMO: 2.09256 factor:1 | 1 (-0.85114) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.75769 HOMO: -6.14977 LUMO: 2.28031 factor:1 | 1 (-1.18370) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.36941 HOMO: -6.70489 LUMO: 2.43814 factor:1 | 1 (-1.79541) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.33969 HOMO: -6.78924 LUMO: 2.27215 factor:1 | 1 (-1.76569) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98698 HOMO: -6.86271 LUMO: 2.31025 factor:1 | 1 (-1.41298) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.95987 HOMO: -6.51168 LUMO: 2.04630 factor:1 | 1 (-1.38588) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.18333 HOMO: -6.72665 LUMO: 2.13337 factor:1 | 1 (-1.60934) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.16325 HOMO: -6.45998 LUMO: 2.16058 factor:1 | 1 (-1.58925) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.07805 HOMO: -6.83822 LUMO: 2.20684 factor:1 | 1 (-2.50405) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.33126 HOMO: -6.68856 LUMO: 2.19324 factor:1 | 1 (-1.75726) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10579 HOMO: -6.71577 LUMO: 2.16058 factor:1 | 1 (-0.53179) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67334 HOMO: -6.82462 LUMO: 1.90208 factor:1 | 1 (-1.09934) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.46812 HOMO: -6.61509 LUMO: 2.23950 factor:1 | 1 (-2.89412) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.17108 HOMO: -6.73754 LUMO: 1.84221 factor:1 | 1 (-2.59708) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01696 HOMO: -6.56611 LUMO: 1.94561 factor:1 | 1 (-1.44297) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99601 HOMO: -6.67767 LUMO: 1.51840 factor:1 | 1 (-1.42201) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17895 HOMO: -6.35658 LUMO: 2.16603 factor:1 | 1 (-1.60495) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51220 HOMO: -6.35114 LUMO: 2.08983 factor:1 | -1 (0.06180) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17672 HOMO: -6.35114 LUMO: 2.10616 factor:1 | 1 (-1.60272) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.05786 HOMO: -6.71305 LUMO: 2.01636 factor:1 | 1 (-1.48386) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42713 HOMO: -6.24773 LUMO: 1.98915 factor:1 | 1 (-0.85313) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60632 HOMO: -6.53617 LUMO: 2.42726 factor:1 | 1 (-1.03232) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.50655 HOMO: -6.59332 LUMO: 1.82316 factor:1 | 1 (-1.93255) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.39354 HOMO: -6.41372 LUMO: 1.77418 factor:1 | 1 (-1.81954) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.19759 HOMO: -6.40284 LUMO: 1.88575 factor:1 | 1 (-1.62359) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.62076 HOMO: -6.11168 LUMO: 1.70888 factor:1 | 1 (-2.04676) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47187 HOMO: -6.44910 LUMO: 2.23405 factor:1 | 1 (-0.89787) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19066 HOMO: -6.24773 LUMO: 2.12793 factor:1 | 1 (-0.61666) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24095 HOMO: -6.07358 LUMO: 1.89663 factor:1 | 1 (-0.66695) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19317 HOMO: -6.66679 LUMO: 1.96738 factor:1 | 1 (-0.61917) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21839 HOMO: -6.68312 LUMO: 1.78235 factor:1 | 1 (-0.64439) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01887 HOMO: -6.70761 LUMO: 1.97555 factor:1 | 1 (-1.44487) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.07705 HOMO: -6.15794 LUMO: 2.00548 factor:1 | 1 (-1.50305) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.95448 HOMO: -6.52257 LUMO: 1.96738 factor:1 | -1 (0.61952) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26534 HOMO: -6.25590 LUMO: 1.86670 factor:1 | -1 (0.30866) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98775 HOMO: -6.30216 LUMO: 1.84765 factor:1 | 1 (-0.41375) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29911 HOMO: -6.76747 LUMO: 2.20956 factor:1 | -1 (0.27489) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.83671 HOMO: -6.14161 LUMO: 1.80684 factor:1 | -1 (0.73729) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62899 HOMO: -6.81373 LUMO: 1.91024 factor:1 | 1 (-0.05499) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87455 HOMO: -6.81917 LUMO: 2.34834 factor:1 | 1 (-0.30055) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68018 HOMO: -6.72121 LUMO: 1.90208 factor:1 | 1 (-0.10618) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10666 HOMO: -7.51851 LUMO: 0.26939 factor:1 | 1 (-0.53266) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.40180 HOMO: -6.65318 LUMO: -0.57144 factor:1 | 1 (-0.82780) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86576 HOMO: -6.77564 LUMO: -0.72654 factor:1 | 1 (-0.29176) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68651 HOMO: -6.80557 LUMO: -0.60954 factor:1 | 1 (-1.11251) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.21656 HOMO: -7.35524 LUMO: 0.27483 factor:1 | 1 (-1.64256) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.15784 HOMO: -6.94979 LUMO: -0.83811 factor:1 | 1 (-1.58384) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.09008 HOMO: -6.13345 LUMO: -0.67212 factor:1 | 1 (-1.51608) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99903 HOMO: -6.47359 LUMO: -0.59321 factor:1 | 1 (-1.42503) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.18442 HOMO: -6.52257 LUMO: -0.54695 factor:1 | -1 (1.38958) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.93889 HOMO: -6.61781 LUMO: -0.69661 factor:1 | -1 (0.63511) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.93965 HOMO: -6.77564 LUMO: -0.80001 factor:1 | -1 (0.63435) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87068 HOMO: -7.35252 LUMO: -1.00410 factor:1 | 1 (-0.29669) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85805 HOMO: -6.35386 LUMO: -0.38912 factor:1 | 1 (-1.28405) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.79785 HOMO: -6.80285 LUMO: -0.52246 factor:1 | -1 (0.77615) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.88759 HOMO: -7.23279 LUMO: 0.30477 factor:1 | -1 (0.68641) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.73970 HOMO: -7.13483 LUMO: -0.76192 factor:1 | -1 (0.83430) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62788 HOMO: -6.71849 LUMO: -0.48164 factor:1 | 1 (-0.05388) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65493 HOMO: -6.85455 LUMO: -0.69389 factor:1 | 1 (-0.08093) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36931 HOMO: -6.96339 LUMO: -0.73743 factor:1 | 1 (-0.79531) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52815 HOMO: -7.50490 LUMO: 0.28844 factor:1 | -1 (0.04585) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62580 HOMO: -6.63958 LUMO: -0.50069 factor:1 | 1 (-1.05180) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73152 HOMO: -6.78924 LUMO: -0.69661 factor:1 | 1 (-1.15752) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.41722 HOMO: -7.44776 LUMO: 0.33742 factor:1 | 1 (-1.84322) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.18065 HOMO: -6.15249 LUMO: 0.66396 factor:1 | 1 (-0.60665) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.33890 HOMO: -6.17426 LUMO: 0.55511 factor:1 | 1 (-1.76490) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.38086 HOMO: -6.83550 LUMO: 0.28844 factor:1 | 1 (-1.80686) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11401 HOMO: -6.32393 LUMO: 0.47620 factor:1 | 1 (-0.54001) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54623 HOMO: -6.32937 LUMO: 0.45987 factor:1 | 1 (-0.97224) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.17703 HOMO: -7.37429 LUMO: 0.09252 factor:1 | 1 (-0.60303) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81302 HOMO: -6.54434 LUMO: -0.39729 factor:1 | 1 (-0.23902) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92657 HOMO: -7.35524 LUMO: 0.28028 factor:1 | 1 (-1.35257) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99930 HOMO: -6.95523 LUMO: -0.86804 factor:1 | 1 (-1.42531) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.12765 HOMO: -6.63958 LUMO: -0.65307 factor:1 | -1 (0.44635) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96021 HOMO: -6.73482 LUMO: -0.67212 factor:1 | 1 (-0.38621) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74755 HOMO: -6.37835 LUMO: -0.53606 factor:1 | 1 (-0.17355) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73934 HOMO: -6.71849 LUMO: -0.61226 factor:1 | 1 (-0.16534) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94799 HOMO: -6.68584 LUMO: -1.11022 factor:1 | 1 (-0.37399) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79422 HOMO: -6.80285 LUMO: -0.79185 factor:1 | 1 (-0.22022) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49731 HOMO: -7.14571 LUMO: -0.94696 factor:1 | 1 (-0.92331) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.67892 HOMO: -7.16204 LUMO: -0.66124 factor:1 | -1 (1.89508) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45135 HOMO: -6.54978 LUMO: -0.54967 factor:1 | 1 (-0.87735) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74056 HOMO: -6.75114 LUMO: -0.70750 factor:1 | 1 (-0.16656) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63920 HOMO: -7.22190 LUMO: 0.39184 factor:1 | 1 (-0.06520) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.07188 HOMO: -7.43959 LUMO: 0.30477 factor:1 | 1 (-1.49788) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.70149 HOMO: -6.87360 LUMO: -0.77552 factor:1 | 1 (-2.12750) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.88224 HOMO: -6.82734 LUMO: -0.59593 factor:1 | 1 (-1.30824) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42610 HOMO: -6.65318 LUMO: -0.46259 factor:1 | 1 (-0.85210) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.27283 HOMO: -7.05863 LUMO: -1.17009 factor:1 | 1 (-1.69883) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61187 HOMO: -6.57427 LUMO: -0.48708 factor:1 | 1 (-1.03787) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49497 HOMO: -6.60420 LUMO: -0.38096 factor:1 | 1 (-0.92097) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.29185 HOMO: -6.72121 LUMO: -0.66668 factor:1 | 1 (-1.71785) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.32549 HOMO: -6.52257 LUMO: -0.19320 factor:1 | 1 (-1.75149) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.42358 HOMO: -6.28039 LUMO: -0.27211 factor:1 | 1 (-1.84959) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47080 HOMO: -6.71849 LUMO: -0.42722 factor:1 | 1 (-0.89681) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.02594 HOMO: -6.27495 LUMO: 0.27756 factor:1 | 1 (-1.45195) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.13025 HOMO: -6.21780 LUMO: 0.46531 factor:1 | 1 (-1.55625) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.70231 HOMO: -6.52257 LUMO: -0.64491 factor:1 | 1 (-2.12831) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.13759 HOMO: -6.73754 LUMO: 1.83133 factor:1 | 1 (-1.56359) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43012 HOMO: -6.67223 LUMO: 1.88847 factor:1 | 1 (-0.85612) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73930 HOMO: -6.82189 LUMO: 1.59187 factor:1 | 1 (-1.16530) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69369 HOMO: -6.43277 LUMO: 1.76330 factor:1 | 1 (-1.11969) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74382 HOMO: -6.48175 LUMO: 1.77962 factor:1 | 1 (-1.16982) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.73276 HOMO: -6.50352 LUMO: 1.68438 factor:1 | 1 (-2.15876) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78943 HOMO: -6.31576 LUMO: 2.03813 factor:1 | 1 (-0.21543) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69838 HOMO: -6.27495 LUMO: 1.99459 factor:1 | 1 (-0.12438) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52183 HOMO: -6.23957 LUMO: 2.17147 factor:1 | 1 (-0.94783) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89515 HOMO: -6.78108 LUMO: 2.16875 factor:1 | 1 (-0.32115) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89869 HOMO: -6.34297 LUMO: 2.10344 factor:1 | 1 (-0.32469) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84265 HOMO: -6.30216 LUMO: 2.00004 factor:1 | 1 (-1.26865) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57500 HOMO: -6.72665 LUMO: 2.09528 factor:1 | 1 (-1.00100) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15053 HOMO: -6.86543 LUMO: 1.91568 factor:1 | 1 (-0.57653) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12930 HOMO: -5.83956 LUMO: 1.89391 factor:1 | 1 (-0.55530) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.09634 HOMO: -6.42189 LUMO: 2.03269 factor:1 | 1 (-1.52234) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13967 HOMO: -6.07630 LUMO: 1.80956 factor:1 | 1 (-0.56567) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03901 HOMO: -6.43277 LUMO: 1.81772 factor:1 | 1 (-0.46502) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93400 HOMO: -7.03959 LUMO: 1.78779 factor:1 | 1 (-1.36000) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74812 HOMO: -6.72121 LUMO: 2.29664 factor:1 | 1 (-0.17413) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63672 HOMO: -6.62869 LUMO: 2.04630 factor:1 | 1 (-0.06272) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.89530 HOMO: -6.63958 LUMO: 1.84221 factor:1 | -1 (1.67870) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77901 HOMO: -6.70761 LUMO: 1.67350 factor:1 | 1 (-0.20501) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86007 HOMO: -6.00283 LUMO: 1.64357 factor:1 | 1 (-0.28607) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72102 HOMO: -6.48719 LUMO: 1.70343 factor:1 | 1 (-0.14702) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81384 HOMO: -6.13345 LUMO: 1.44492 factor:1 | 1 (-0.23984) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86941 HOMO: -6.11168 LUMO: 1.70071 factor:1 | 1 (-0.29541) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76168 HOMO: -6.09535 LUMO: 1.82316 factor:1 | 1 (-0.18768) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80998 HOMO: -6.81101 LUMO: 1.63540 factor:1 | 1 (-0.23598) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54823 HOMO: -6.80013 LUMO: 2.12249 factor:1 | -1 (0.02577) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93771 HOMO: -6.48447 LUMO: 1.94561 factor:1 | 1 (-0.36371) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73438 HOMO: -6.72393 LUMO: 2.06534 factor:1 | 1 (-0.16038) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65588 HOMO: -6.34570 LUMO: 1.98915 factor:1 | 1 (-0.08188) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83648 HOMO: -6.31304 LUMO: 1.87759 factor:1 | 1 (-0.26248) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77852 HOMO: -6.77564 LUMO: 1.81228 factor:1 | 1 (-0.20452) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85776 HOMO: -6.58516 LUMO: 2.34834 factor:1 | 1 (-0.28376) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77817 HOMO: -6.68040 LUMO: 2.20412 factor:1 | 1 (-0.20417) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91175 HOMO: -6.20964 LUMO: 2.17147 factor:1 | 1 (-0.33775) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64742 HOMO: -6.54706 LUMO: 2.03813 factor:1 | 1 (-0.07342) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67952 HOMO: -6.54162 LUMO: 2.17419 factor:1 | 1 (-0.10553) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76369 HOMO: -6.75659 LUMO: 2.22589 factor:1 | 1 (-0.18969) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43195 HOMO: -6.59604 LUMO: 2.59325 factor:1 | 1 (-0.85795) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54316 HOMO: -6.11712 LUMO: 2.02181 factor:1 | 1 (-0.96916) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36933 HOMO: -6.63141 LUMO: 2.09256 factor:1 | 1 (-0.79533) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29037 HOMO: -6.61781 LUMO: 1.86126 factor:1 | 1 (-0.71637) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80821 HOMO: -6.63958 LUMO: 1.77146 factor:1 | 1 (-0.23421) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80875 HOMO: -6.60420 LUMO: 1.54561 factor:1 | 1 (-0.23475) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80198 HOMO: -6.52529 LUMO: 2.05174 factor:1 | 1 (-0.22798) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62295 HOMO: -6.80285 LUMO: 2.13609 factor:1 | 1 (-0.04895) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08303 HOMO: -6.51168 LUMO: 2.25855 factor:1 | 1 (-1.50903) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77497 HOMO: -6.64774 LUMO: 2.46263 factor:1 | 1 (-1.20097) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91425 HOMO: -6.40828 LUMO: 1.99732 factor:1 | 1 (-0.34025) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68638 HOMO: -5.97562 LUMO: 1.56465 factor:1 | 1 (-0.11238) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.37871 HOMO: -6.75659 LUMO: 2.23405 factor:1 | 1 (-1.80471) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79568 HOMO: -6.68584 LUMO: 2.09528 factor:1 | 1 (-1.22168) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90445 HOMO: -6.86543 LUMO: 1.95106 factor:1 | 1 (-0.33046) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71735 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-0.14335) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.25898 HOMO: -6.87632 LUMO: 2.08439 factor:1 | 1 (-1.68498) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74556 HOMO: -6.33753 LUMO: 2.16603 factor:1 | 1 (-1.17156) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.37742 HOMO: -6.92258 LUMO: 1.72248 factor:1 | 1 (-0.80342) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79304 HOMO: -6.62597 LUMO: 2.10344 factor:1 | 1 (-1.21904) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.21599 HOMO: -6.63141 LUMO: 1.94017 factor:1 | 1 (-1.64199) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35388 HOMO: -6.48447 LUMO: 1.91840 factor:1 | 1 (-0.77988) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68025 HOMO: -6.41372 LUMO: 1.61364 factor:1 | 1 (-1.10625) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82813 HOMO: -6.37291 LUMO: 1.79051 factor:1 | 1 (-0.25413) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.91701 HOMO: -6.13073 LUMO: 1.77962 factor:1 | -1 (0.65699) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24710 HOMO: -6.13073 LUMO: 1.98915 factor:1 | 1 (-0.67310) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.37412 HOMO: -6.44094 LUMO: 1.58370 factor:1 | 1 (-0.80012) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94026 HOMO: -6.87087 LUMO: -0.82995 factor:1 | 1 (-0.36627) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.00381 HOMO: -6.67223 LUMO: 1.08029 factor:1 | -1 (0.57019) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94602 HOMO: -6.82462 LUMO: 0.91702 factor:1 | 1 (-1.37203) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99525 HOMO: -6.65863 LUMO: 1.52656 factor:1 | 1 (-1.42125) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66638 HOMO: -6.78924 LUMO: 0.86260 factor:1 | 1 (-0.09238) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.50416 HOMO: -6.68584 LUMO: 0.94424 factor:1 | 1 (-1.93016) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85936 HOMO: -6.58788 LUMO: 1.00138 factor:1 | 1 (-0.28537) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.14196 HOMO: -6.79740 LUMO: 0.91430 factor:1 | -1 (0.43204) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.15830 HOMO: -6.67223 LUMO: 0.80274 factor:1 | 1 (-1.58430) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02761 HOMO: -6.95251 LUMO: 0.90614 factor:1 | 1 (-0.45361) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09771 HOMO: -7.19469 LUMO: 1.34152 factor:1 | 1 (-0.52371) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08691 HOMO: -6.59332 LUMO: -0.76464 factor:1 | 1 (-0.51291) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02310 HOMO: -6.77564 LUMO: -0.90886 factor:1 | 1 (-0.44910) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97977 HOMO: -6.57971 LUMO: -0.41633 factor:1 | 1 (-1.40577) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57745 HOMO: -6.68856 LUMO: -0.58232 factor:1 | 1 (-0.00346) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70001 HOMO: -6.87087 LUMO: -0.71022 factor:1 | 1 (-0.12602) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53785 HOMO: -6.67767 LUMO: -0.74559 factor:1 | 1 (-0.96385) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59579 HOMO: -6.68040 LUMO: -0.65307 factor:1 | 1 (-1.02179) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66776 HOMO: -6.32937 LUMO: 0.80274 factor:1 | 1 (-1.09376) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.71780 HOMO: -6.29671 LUMO: 0.82723 factor:1 | 1 (-1.14380) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77666 HOMO: -6.67767 LUMO: 0.59321 factor:1 | 1 (-1.20266) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.10782 HOMO: -6.77836 LUMO: 0.50341 factor:1 | 1 (-1.53382) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62180 HOMO: -6.61781 LUMO: 0.42450 factor:1 | 1 (-1.04780) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77281 HOMO: -6.83278 LUMO: 0.39457 factor:1 | 1 (-0.19881) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.82403 HOMO: -6.56883 LUMO: 0.64219 factor:1 | -1 (0.74997) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85683 HOMO: -6.71577 LUMO: 0.40001 factor:1 | 1 (-0.28284) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99406 HOMO: -6.86543 LUMO: -0.74287 factor:1 | 1 (-0.42006) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90228 HOMO: -6.68584 LUMO: -0.69389 factor:1 | 1 (-0.32828) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00157 HOMO: -6.61237 LUMO: -0.48980 factor:1 | 1 (-0.42757) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92353 HOMO: -6.80285 LUMO: -0.58232 factor:1 | 1 (-0.34953) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89430 HOMO: -6.88992 LUMO: -0.70205 factor:1 | 1 (-0.32031) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73667 HOMO: -6.95251 LUMO: -0.71838 factor:1 | 1 (-0.16267) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.37430 HOMO: -7.52123 LUMO: 0.27211 factor:1 | -1 (1.19970) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.33326 HOMO: -6.76747 LUMO: -0.74015 factor:1 | -1 (0.24074) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.25032 HOMO: -6.55250 LUMO: -0.49797 factor:1 | -1 (0.32368) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82883 HOMO: -6.50896 LUMO: -0.46804 factor:1 | 1 (-0.25483) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55664 HOMO: -7.45320 LUMO: 0.08436 factor:1 | -1 (0.01736) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.00802 HOMO: -6.82462 LUMO: -0.70477 factor:1 | -1 (2.56598) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.97956 HOMO: -6.57155 LUMO: -0.43538 factor:1 | -1 (2.59444) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85566 HOMO: -6.72665 LUMO: -0.55239 factor:1 | 1 (-0.28167) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82111 HOMO: -7.05319 LUMO: -1.08573 factor:1 | 1 (-0.24711) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19070 HOMO: -6.56067 LUMO: -0.45715 factor:1 | -1 (0.38330) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.24760 HOMO: -6.76475 LUMO: -0.53879 factor:1 | -1 (0.32640) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.25402 HOMO: -6.67223 LUMO: -0.45987 factor:1 | -1 (0.31998) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.28850 HOMO: -6.44094 LUMO: -0.72110 factor:1 | -1 (0.28550) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86097 HOMO: -6.66951 LUMO: -0.67756 factor:1 | 1 (-0.28697) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.68295 HOMO: -6.69400 LUMO: -0.62858 factor:1 | -1 (2.89105) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.74304 HOMO: -6.51985 LUMO: -0.37007 factor:1 | -1 (2.83096) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.15776 HOMO: -5.98378 LUMO: 0.78641 factor:1 | 1 (-1.58376) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.71601 HOMO: -6.11440 LUMO: 0.71294 factor:1 | 1 (-1.14201) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.40549 HOMO: -6.45182 LUMO: 0.63947 factor:1 | 1 (-1.83149) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81624 HOMO: -6.78924 LUMO: 0.37007 factor:1 | -1 (0.75776) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02459 HOMO: -6.63686 LUMO: 0.54423 factor:1 | 1 (-0.45059) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.88699 HOMO: -6.66679 LUMO: 0.48708 factor:1 | 1 (-2.31300) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.33482 HOMO: -6.81917 LUMO: 0.31021 factor:1 | 1 (-1.76082) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.32785 HOMO: -6.28583 LUMO: 0.44899 factor:1 | 1 (-1.75386) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.52906 HOMO: -6.61237 LUMO: 0.49525 factor:1 | 1 (-1.95506) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83982 HOMO: -7.08857 LUMO: 0.38368 factor:1 | 1 (-1.26582) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89757 HOMO: -6.53890 LUMO: -0.68845 factor:1 | 1 (-0.32357) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.39810 HOMO: -6.56611 LUMO: -0.66396 factor:1 | -1 (0.17589) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.03189 HOMO: -6.04909 LUMO: -0.59865 factor:1 | -1 (0.54211) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67563 HOMO: -6.74842 LUMO: -0.77825 factor:1 | 1 (-0.10163) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05257 HOMO: -6.82462 LUMO: -0.61498 factor:1 | -1 (0.52142) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.31885 HOMO: -7.40694 LUMO: 0.32926 factor:1 | -1 (1.25515) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.61013 HOMO: -6.80557 LUMO: -0.57416 factor:1 | -1 (1.96387) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.42893 HOMO: -6.76747 LUMO: -0.67484 factor:1 | -1 (0.14506) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.10825 HOMO: -7.23279 LUMO: 0.48980 factor:1 | -1 (0.46575) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.02814 HOMO: -6.62869 LUMO: -0.24762 factor:1 | -1 (0.54586) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.57012 HOMO: -6.65863 LUMO: -0.28028 factor:1 | -1 (1.00388) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66429 HOMO: -6.50352 LUMO: -0.44899 factor:1 | 1 (-0.09029) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.58878 HOMO: -6.62053 LUMO: -0.88437 factor:1 | 1 (-2.01479) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.25076 HOMO: -6.73754 LUMO: -0.77825 factor:1 | 1 (-1.67677) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.32108 HOMO: -7.24639 LUMO: 0.35647 factor:1 | 1 (-1.74708) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62066 HOMO: -6.46270 LUMO: -0.48164 factor:1 | 1 (-1.04666) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91572 HOMO: -6.14161 LUMO: -0.66396 factor:1 | 1 (-0.34172) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91994 HOMO: -6.63414 LUMO: 1.51295 factor:1 | 1 (-0.34594) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88892 HOMO: -6.52529 LUMO: 1.65989 factor:1 | 1 (-0.31492) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82089 HOMO: -6.63686 LUMO: 1.64629 factor:1 | 1 (-0.24689) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63182 HOMO: -6.49808 LUMO: 1.60003 factor:1 | 1 (-0.05782) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87286 HOMO: -6.85183 LUMO: 1.96194 factor:1 | 1 (-0.29886) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16359 HOMO: -6.90081 LUMO: 1.82316 factor:1 | 1 (-0.58959) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31227 HOMO: -6.20147 LUMO: 1.95106 factor:1 | 1 (-0.73827) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.19779 HOMO: -7.05047 LUMO: 1.94289 factor:1 | -1 (2.37621) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.72182 HOMO: -6.11440 LUMO: 1.83949 factor:1 | 1 (-2.14782) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06009 HOMO: -6.65046 LUMO: 1.59187 factor:1 | 1 (-1.48610) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39420 HOMO: -6.81917 LUMO: 2.41365 factor:1 | 1 (-0.82021) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73775 HOMO: -6.40284 LUMO: 2.48984 factor:1 | 1 (-1.16375) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71705 HOMO: -7.04775 LUMO: 2.31025 factor:1 | 1 (-0.14305) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77743 HOMO: -6.64774 LUMO: 2.20140 factor:1 | 1 (-0.20343) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.27028 HOMO: -6.72393 LUMO: 2.28304 factor:1 | 1 (-1.69628) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48525 HOMO: -6.35114 LUMO: 1.84765 factor:1 | 1 (-0.91125) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80191 HOMO: -6.41100 LUMO: 1.74697 factor:1 | 1 (-1.22791) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95697 HOMO: -6.34297 LUMO: 1.55921 factor:1 | 1 (-0.38297) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.17851 HOMO: -6.31848 LUMO: 1.67622 factor:1 | -1 (0.39549) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74927 HOMO: -6.50896 LUMO: 2.02725 factor:1 | 1 (-0.17527) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.40961 HOMO: -6.28583 LUMO: 2.00548 factor:1 | -1 (0.16438) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.23616 HOMO: -6.67495 LUMO: 1.92384 factor:1 | 1 (-0.66216) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51568 HOMO: -6.17154 LUMO: 2.39732 factor:1 | -1 (0.05831) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.41495 HOMO: -6.84911 LUMO: 2.24766 factor:1 | -1 (0.15905) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09308 HOMO: -6.77564 LUMO: 2.38372 factor:1 | 1 (-0.51908) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.32348 HOMO: -6.18243 LUMO: 2.40821 factor:1 | 1 (-0.74948) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.25000 HOMO: -6.40828 LUMO: 2.22589 factor:1 | 1 (-1.67600) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69720 HOMO: -6.74570 LUMO: 1.88303 factor:1 | 1 (-1.12320) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65064 HOMO: -6.29944 LUMO: 2.05174 factor:1 | 1 (-1.07665) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84200 HOMO: -7.00693 LUMO: 2.16331 factor:1 | 1 (-0.26800) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55200 HOMO: -6.89537 LUMO: 2.19596 factor:1 | 1 (-0.97800) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.83647 HOMO: -6.72665 LUMO: 2.03813 factor:1 | -1 (1.73753) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.22480 HOMO: -6.69944 LUMO: 2.36467 factor:1 | -1 (0.34920) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94901 HOMO: -6.92802 LUMO: 1.72792 factor:1 | -1 (0.62499) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.80612 HOMO: -6.12256 LUMO: 1.85310 factor:1 | -1 (0.76788) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89819 HOMO: -6.70489 LUMO: 2.20956 factor:1 | 1 (-1.32419) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.71391 HOMO: -6.94707 LUMO: 1.81500 factor:1 | 1 (-1.13991) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.47262 HOMO: -6.39468 LUMO: 1.79051 factor:1 | -1 (1.10138) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.70452 HOMO: -6.69128 LUMO: 2.03813 factor:1 | -1 (1.86948) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15334 HOMO: -6.55250 LUMO: 2.00548 factor:1 | -1 (0.42066) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.61635 HOMO: -6.24773 LUMO: 2.09256 factor:1 | -1 (0.95765) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36639 HOMO: -6.85727 LUMO: 1.70071 factor:1 | 1 (-0.79240) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93990 HOMO: -6.71305 LUMO: 1.72520 factor:1 | 1 (-1.36590) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90905 HOMO: -6.81101 LUMO: 2.15514 factor:1 | 1 (-0.33505) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73500 HOMO: -6.93618 LUMO: 1.75513 factor:1 | 1 (-1.16100) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96677 HOMO: -6.63686 LUMO: 2.09800 factor:1 | 1 (-0.39277) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76510 HOMO: -6.98244 LUMO: 1.72520 factor:1 | 1 (-0.19111) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61914 HOMO: -6.37019 LUMO: 2.35923 factor:1 | 1 (-0.04514) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48408 HOMO: -6.55794 LUMO: 2.12521 factor:1 | 1 (-0.91008) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35865 HOMO: -6.45998 LUMO: 1.93201 factor:1 | -1 (0.21535) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.70394 HOMO: -6.71033 LUMO: 1.58370 factor:1 | -1 (0.87006) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.77877 HOMO: -6.67223 LUMO: 1.52928 factor:1 | -1 (0.79523) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.68726 HOMO: -6.72121 LUMO: 1.33608 factor:1 | -1 (0.88674) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69715 HOMO: -6.89264 LUMO: 2.08983 factor:1 | 1 (-1.12315) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.96121 HOMO: -6.31032 LUMO: 2.24766 factor:1 | 1 (-1.38721) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28849 HOMO: -6.79740 LUMO: 2.09528 factor:1 | 1 (-0.71449) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08095 HOMO: -6.78108 LUMO: 2.15786 factor:1 | 1 (-0.50695) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92918 HOMO: -6.50896 LUMO: 2.15786 factor:1 | 1 (-1.35518) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83348 HOMO: -6.56067 LUMO: 2.24494 factor:1 | 1 (-1.25948) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67399 HOMO: -6.72938 LUMO: 2.24494 factor:1 | 1 (-1.09999) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21649 HOMO: -6.40556 LUMO: 1.58642 factor:1 | 1 (-0.64249) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63214 HOMO: -6.63141 LUMO: 1.66262 factor:1 | 1 (-1.05814) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84170 HOMO: -6.97156 LUMO: 2.23678 factor:1 | 1 (-1.26770) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91697 HOMO: -6.86271 LUMO: 1.91296 factor:1 | 1 (-0.34297) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86677 HOMO: -6.50624 LUMO: 1.89119 factor:1 | 1 (-0.29277) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84549 HOMO: -6.70761 LUMO: 1.56193 factor:1 | 1 (-0.27149) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74992 HOMO: -6.60420 LUMO: 1.79595 factor:1 | 1 (-0.17592) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80442 HOMO: -6.85727 LUMO: 2.26943 factor:1 | 1 (-0.23043) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60839 HOMO: -6.23413 LUMO: 1.91024 factor:1 | 1 (-0.03440) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.07977 HOMO: -6.84366 LUMO: 2.01364 factor:1 | 1 (-1.50577) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63334 HOMO: -6.63414 LUMO: 2.54971 factor:1 | 1 (-1.05934) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.83224 HOMO: -6.52257 LUMO: 2.42998 factor:1 | 1 (-2.25825) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62687 HOMO: -6.61509 LUMO: 2.31297 factor:1 | 1 (-0.05287) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22250 HOMO: -6.45998 LUMO: 2.23405 factor:1 | 1 (-0.64850) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.23066 HOMO: -6.86271 LUMO: 2.22317 factor:1 | 1 (-0.65667) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78704 HOMO: -6.84366 LUMO: 2.11432 factor:1 | 1 (-0.21304) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65957 HOMO: -6.85999 LUMO: 2.44902 factor:1 | 1 (-1.08557) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86028 HOMO: -6.73482 LUMO: 1.93745 factor:1 | 1 (-1.28628) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52218 HOMO: -6.91441 LUMO: 2.32385 factor:1 | 1 (-0.94818) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53076 HOMO: -6.16066 LUMO: 2.26399 factor:1 | -1 (0.04324) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75340 HOMO: -6.71305 LUMO: 2.38644 factor:1 | 1 (-0.17940) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74176 HOMO: -7.08312 LUMO: 2.01636 factor:1 | 1 (-0.16776) | 1 | 1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43849 HOMO: -6.15249 LUMO: 1.90752 factor:1 | -1 (0.13551) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77792 HOMO: -6.83006 LUMO: 2.25855 factor:1 | 1 (-0.20392) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68521 HOMO: -6.77836 LUMO: 2.24766 factor:1 | 1 (-0.11121) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35340 HOMO: -6.66951 LUMO: 2.35923 factor:1 | -1 (0.22060) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69381 HOMO: -6.68312 LUMO: 2.30208 factor:1 | 1 (-0.11981) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51683 HOMO: -6.49808 LUMO: 2.49801 factor:1 | -1 (0.05717) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65266 HOMO: -6.62325 LUMO: 1.89935 factor:1 | 1 (-1.07866) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57764 HOMO: -6.80829 LUMO: 1.91296 factor:1 | 1 (-1.00364) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79006 HOMO: -6.64230 LUMO: 2.13065 factor:1 | 1 (-0.21606) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89341 HOMO: -6.40556 LUMO: 1.83949 factor:1 | -1 (0.68058) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.30056 HOMO: -6.48175 LUMO: 1.72248 factor:1 | 1 (-1.72656) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.19267 HOMO: -6.61781 LUMO: 2.11432 factor:1 | 1 (-1.61867) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89417 HOMO: -6.34570 LUMO: 2.22317 factor:1 | 1 (-0.32017) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83901 HOMO: -7.00149 LUMO: 1.80139 factor:1 | 1 (-0.26501) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68009 HOMO: -6.66951 LUMO: 2.13065 factor:1 | 1 (-1.10609) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19798 HOMO: -6.54434 LUMO: 2.20140 factor:1 | 1 (-0.62398) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11219 HOMO: -6.67767 LUMO: 2.02997 factor:1 | 1 (-0.53819) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.34752 HOMO: -6.49536 LUMO: 2.42998 factor:1 | -1 (0.22648) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73085 HOMO: -6.70761 LUMO: 2.71025 factor:1 | 1 (-0.15685) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39222 HOMO: -6.62869 LUMO: 2.11160 factor:1 | 1 (-0.81822) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.36492 HOMO: -6.61781 LUMO: 2.24494 factor:1 | 1 (-1.79092) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73617 HOMO: -6.66135 LUMO: 2.20956 factor:1 | 1 (-1.16217) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.20730 HOMO: -6.95523 LUMO: 2.03813 factor:1 | -1 (0.36670) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00205 HOMO: -7.11578 LUMO: 2.41365 factor:1 | 1 (-1.42805) | 1 | 1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03455 HOMO: -6.99061 LUMO: 2.13881 factor:1 | 1 (-0.46055) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.71205 HOMO: -6.43277 LUMO: 2.01364 factor:1 | 1 (-2.13805) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54041 HOMO: -6.79196 LUMO: 2.04358 factor:1 | 1 (-0.96641) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93711 HOMO: -7.08584 LUMO: 1.99732 factor:1 | 1 (-0.36311) | 1 | 1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59486 HOMO: -6.46815 LUMO: 2.29936 factor:1 | 1 (-1.02086) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76140 HOMO: -6.78108 LUMO: 1.93745 factor:1 | 1 (-0.18740) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03910 HOMO: -6.43277 LUMO: 1.80956 factor:1 | 1 (-0.46510) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10204 HOMO: -6.71577 LUMO: -0.81090 factor:1 | 1 (-0.52804) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.34931 HOMO: -7.14027 LUMO: -0.68028 factor:1 | -1 (0.22468) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61495 HOMO: -7.03414 LUMO: -0.69661 factor:1 | 1 (-0.04095) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.37231 HOMO: -6.64502 LUMO: -0.47348 factor:1 | -1 (0.20169) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52681 HOMO: -6.60692 LUMO: 2.12793 factor:1 | 1 (-0.95281) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.22266 HOMO: -6.66407 LUMO: 1.94561 factor:1 | 1 (-1.64866) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70210 HOMO: -7.10217 LUMO: 1.92384 factor:1 | 1 (-1.12810) | 1 | 1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78440 HOMO: -6.84094 LUMO: 1.66534 factor:1 | 1 (-0.21040) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.85358 HOMO: -6.93618 LUMO: 2.13065 factor:1 | -1 (0.72042) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38313 HOMO: -6.60692 LUMO: 2.20684 factor:1 | 1 (-0.80913) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54961 HOMO: -6.85727 LUMO: 2.19324 factor:1 | 1 (-0.97561) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83114 HOMO: -6.31032 LUMO: 1.76330 factor:1 | 1 (-1.25714) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.16608 HOMO: -6.43821 LUMO: 2.10072 factor:1 | 1 (-1.59208) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45595 HOMO: -6.42189 LUMO: 2.19596 factor:1 | 1 (-0.88195) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.46672 HOMO: -6.40556 LUMO: 2.02181 factor:1 | 1 (-0.89272) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59108 HOMO: -6.41372 LUMO: 2.26671 factor:1 | 1 (-1.01708) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68127 HOMO: -6.60692 LUMO: 2.09800 factor:1 | 1 (-0.10727) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81720 HOMO: -6.75931 LUMO: 1.76602 factor:1 | -1 (0.75680) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22321 HOMO: -6.39195 LUMO: 1.84221 factor:1 | 1 (-0.64921) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55185 HOMO: -6.74570 LUMO: 2.04085 factor:1 | -1 (0.02215) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38327 HOMO: -6.77019 LUMO: 2.16875 factor:1 | -1 (0.19072) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12236 HOMO: -6.15522 LUMO: 1.81772 factor:1 | 1 (-0.54836) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.27866 HOMO: -6.48175 LUMO: 2.02453 factor:1 | 1 (-1.70466) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.03755 HOMO: -6.57427 LUMO: 1.77962 factor:1 | 1 (-2.46356) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02935 HOMO: -6.57699 LUMO: 2.42998 factor:1 | 1 (-0.45536) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30065 HOMO: -6.35386 LUMO: 2.25310 factor:1 | 1 (-0.72665) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.05884 HOMO: -6.80013 LUMO: 2.11160 factor:1 | 1 (-1.48484) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.34356 HOMO: -6.24229 LUMO: 2.05718 factor:1 | 1 (-0.76957) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01544 HOMO: -6.42733 LUMO: 1.76874 factor:1 | 1 (-1.44144) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44330 HOMO: -6.56883 LUMO: 2.36195 factor:1 | -1 (0.13070) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00568 HOMO: -6.72665 LUMO: 2.28848 factor:1 | 1 (-0.43168) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.05642 HOMO: -6.39195 LUMO: 1.79051 factor:1 | -1 (1.51758) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.39412 HOMO: -6.70761 LUMO: 0.15510 factor:1 | -1 (2.17988) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.27366 HOMO: -6.44366 LUMO: -0.16871 factor:1 | -1 (2.30034) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.10865 HOMO: -6.68584 LUMO: 1.69527 factor:1 | -1 (2.46535) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.95305 HOMO: -6.26950 LUMO: 1.61636 factor:1 | -1 (2.62095) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96048 HOMO: -6.47631 LUMO: 1.98915 factor:1 | 1 (-0.38648) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81414 HOMO: -6.58243 LUMO: 1.97283 factor:1 | 1 (-0.24014) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.21290 HOMO: -6.51713 LUMO: 1.97283 factor:1 | -1 (0.36110) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96685 HOMO: -6.65046 LUMO: 1.69255 factor:1 | 1 (-0.39285) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93893 HOMO: -6.26406 LUMO: 2.21773 factor:1 | 1 (-0.36493) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.30262 HOMO: -6.88992 LUMO: 2.28304 factor:1 | -1 (0.27138) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08616 HOMO: -6.67767 LUMO: 2.34834 factor:1 | 1 (-1.51216) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15959 HOMO: -6.52801 LUMO: 2.10344 factor:1 | 1 (-0.58559) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06721 HOMO: -6.52801 LUMO: 2.24222 factor:1 | 1 (-0.49321) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82910 HOMO: -6.17154 LUMO: 1.89663 factor:1 | 1 (-1.25510) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45639 HOMO: -6.42733 LUMO: 2.15514 factor:1 | -1 (0.11761) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.23397 HOMO: -6.36474 LUMO: 2.01364 factor:1 | -1 (1.34002) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11944.11171 HOMO: -6.82189 LUMO: 1.86942 factor:1 | -1 (4.46229) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11943.99002 HOMO: -6.60148 LUMO: 2.00548 factor:1 | -1 (4.58398) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55375 HOMO: -6.67767 LUMO: 2.15786 factor:1 | -1 (0.02025) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81999 HOMO: -6.79196 LUMO: 2.06534 factor:1 | 1 (-0.24599) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.26498 HOMO: -6.70216 LUMO: 1.83405 factor:1 | 1 (-0.69098) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.07315 HOMO: -6.58788 LUMO: 1.79051 factor:1 | -1 (1.50084) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.08461 HOMO: -6.34842 LUMO: 1.80139 factor:1 | -1 (1.48939) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.13442 HOMO: -6.48175 LUMO: 1.95922 factor:1 | -1 (2.43958) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.91194 HOMO: -6.71033 LUMO: 2.02997 factor:1 | -1 (2.66206) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.60906 HOMO: -6.89264 LUMO: 2.42726 factor:1 | -1 (0.96494) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.08760 HOMO: -6.74570 LUMO: 2.20684 factor:1 | -1 (1.48639) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82062 HOMO: -6.30216 LUMO: 2.15242 factor:1 | 1 (-0.24662) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.77761 HOMO: -6.94979 LUMO: 2.43814 factor:1 | -1 (1.79639) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.92112 HOMO: -6.97972 LUMO: 2.11432 factor:1 | -1 (1.65287) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.76296 HOMO: -6.17154 LUMO: 1.98099 factor:1 | -1 (0.81104) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89722 HOMO: -6.74026 LUMO: 2.21501 factor:1 | -1 (0.67677) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.63684 HOMO: -6.72393 LUMO: 2.19596 factor:1 | -1 (0.93716) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84129 HOMO: -6.11440 LUMO: 2.10072 factor:1 | 1 (-1.26729) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10168 HOMO: -6.34297 LUMO: 1.92657 factor:1 | 1 (-0.52768) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88445 HOMO: -6.24773 LUMO: 2.00276 factor:1 | 1 (-0.31045) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15357 HOMO: -6.75114 LUMO: 1.98643 factor:1 | 1 (-0.57958) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.19854 HOMO: -6.69128 LUMO: 2.08711 factor:1 | -1 (1.37545) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89362 HOMO: -6.65318 LUMO: 2.15514 factor:1 | 1 (-0.31962) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75169 HOMO: -6.67495 LUMO: 1.72248 factor:1 | 1 (-0.17769) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77533 HOMO: -6.58243 LUMO: 1.83405 factor:1 | 1 (-1.20133) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86591 HOMO: -6.61237 LUMO: 1.69799 factor:1 | 1 (-1.29191) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.17406 HOMO: -6.57427 LUMO: 2.29936 factor:1 | 1 (-0.60007) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88358 HOMO: -6.40012 LUMO: 2.35378 factor:1 | 1 (-0.30958) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60894 HOMO: -6.90081 LUMO: 2.26671 factor:1 | 1 (-0.03494) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80668 HOMO: -6.44910 LUMO: 2.25855 factor:1 | 1 (-0.23268) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73489 HOMO: -6.61509 LUMO: 2.26943 factor:1 | 1 (-1.16089) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89982 HOMO: -6.78924 LUMO: 2.09256 factor:1 | 1 (-1.32582) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91043 HOMO: -6.47087 LUMO: 1.97555 factor:1 | 1 (-1.33643) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.32834 HOMO: -6.75931 LUMO: 1.98643 factor:1 | 1 (-1.75435) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49451 HOMO: -6.17971 LUMO: 2.09800 factor:1 | 1 (-0.92051) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.25944 HOMO: -6.83006 LUMO: 1.91840 factor:1 | 1 (-1.68545) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.85396 HOMO: -6.72938 LUMO: 2.17419 factor:1 | 1 (-2.27996) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13521 HOMO: -6.78924 LUMO: 2.42726 factor:1 | 1 (-0.56121) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62325 HOMO: -6.41372 LUMO: 1.93745 factor:1 | 1 (-0.04925) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20680 HOMO: -6.85455 LUMO: 2.14970 factor:1 | 1 (-0.63280) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.41762 HOMO: -6.38651 LUMO: 2.18507 factor:1 | -1 (0.15638) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.53959 HOMO: -6.81373 LUMO: 2.00548 factor:1 | 1 (-1.96559) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.11318 HOMO: -6.64774 LUMO: 2.41365 factor:1 | 1 (-1.53918) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57930 HOMO: -6.70489 LUMO: 2.31569 factor:1 | 1 (-1.00530) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78270 HOMO: -6.49264 LUMO: 1.78779 factor:1 | 1 (-1.20870) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21543 HOMO: -6.81101 LUMO: 1.86670 factor:1 | 1 (-0.64143) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72335 HOMO: -6.72121 LUMO: 1.48846 factor:1 | 1 (-1.14935) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82246 HOMO: -6.35930 LUMO: 1.78507 factor:1 | 1 (-1.24846) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12274 HOMO: -6.38651 LUMO: 2.04358 factor:1 | 1 (-0.54874) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20609 HOMO: -6.42189 LUMO: 1.99187 factor:1 | 1 (-0.63209) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.94705 HOMO: -6.69400 LUMO: 1.61091 factor:1 | 1 (-2.37305) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.73909 HOMO: -6.81101 LUMO: 2.17419 factor:1 | 1 (-3.16509) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.94925 HOMO: -6.90897 LUMO: 2.28576 factor:1 | 1 (-2.37525) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.13587 HOMO: -6.75387 LUMO: 2.31297 factor:1 | 1 (-2.56187) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.48514 HOMO: -7.05863 LUMO: 2.18780 factor:1 | 1 (-1.91114) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.60419 HOMO: -6.56611 LUMO: 1.99187 factor:1 | 1 (-2.03019) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.78125 HOMO: -6.59060 LUMO: 1.86398 factor:1 | 1 (-2.20725) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.46078 HOMO: -6.59060 LUMO: 1.59459 factor:1 | 1 (-1.88678) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10296 HOMO: -6.57699 LUMO: 1.48030 factor:1 | 1 (-0.52896) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.45855 HOMO: -6.99605 LUMO: 2.30208 factor:1 | 1 (-1.88455) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.05473 HOMO: -6.42189 LUMO: 2.20412 factor:1 | 1 (-1.48073) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05444 HOMO: -7.15115 LUMO: 1.83405 factor:1 | 1 (-0.48044) | 1 | 1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12944 HOMO: -7.08040 LUMO: 2.21773 factor:1 | 1 (-0.55544) | 1 | 1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43495 HOMO: -6.72121 LUMO: 1.89663 factor:1 | -1 (0.13905) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12666 HOMO: -6.25590 LUMO: 1.85037 factor:1 | 1 (-0.55266) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80870 HOMO: -6.70489 LUMO: 1.98915 factor:1 | 1 (-0.23470) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.26188 HOMO: -6.53617 LUMO: 2.08439 factor:1 | 1 (-0.68788) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30925 HOMO: -6.69944 LUMO: 1.98915 factor:1 | 1 (-0.73525) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65525 HOMO: -6.79468 LUMO: 1.96466 factor:1 | 1 (-0.08125) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24887 HOMO: -6.79468 LUMO: 1.99459 factor:1 | 1 (-0.67487) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62834 HOMO: -6.58788 LUMO: 1.98371 factor:1 | 1 (-0.05434) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.31707 HOMO: -6.58788 LUMO: 2.16603 factor:1 | -1 (0.25693) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00380 HOMO: -6.56883 LUMO: 1.64085 factor:1 | 1 (-0.42980) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.37861 HOMO: -7.19197 LUMO: 2.66127 factor:1 | 1 (-0.80461) | 1 | 1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02029 HOMO: -6.48175 LUMO: 2.40004 factor:1 | 1 (-0.44629) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48777 HOMO: -6.18515 LUMO: 2.27759 factor:1 | -1 (0.08623) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13405 HOMO: -6.64774 LUMO: 2.13337 factor:1 | -1 (0.43995) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.34880 HOMO: -6.39740 LUMO: 1.95106 factor:1 | -1 (0.22520) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.39459 HOMO: -6.59332 LUMO: 1.81772 factor:1 | -1 (0.17940) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.68664 HOMO: -6.68312 LUMO: 2.41909 factor:1 | -1 (0.88736) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00353 HOMO: -5.87494 LUMO: 2.18235 factor:1 | 1 (-0.42953) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10051 HOMO: -6.30488 LUMO: 2.04902 factor:1 | 1 (-0.52651) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47375 HOMO: -6.65046 LUMO: 2.05446 factor:1 | -1 (0.10025) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22598 HOMO: -6.55794 LUMO: 2.06807 factor:1 | 1 (-0.65198) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59463 HOMO: -6.68040 LUMO: 1.99187 factor:1 | 1 (-0.02063) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72864 HOMO: -6.60965 LUMO: 2.18780 factor:1 | 1 (-0.15464) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10759 HOMO: -6.88176 LUMO: 2.10344 factor:1 | 1 (-0.53359) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20397 HOMO: -6.63414 LUMO: 1.70615 factor:1 | 1 (-0.62997) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61264 HOMO: -7.15115 LUMO: 2.07351 factor:1 | 1 (-0.03864) | 1 | 1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.10577 HOMO: -6.85727 LUMO: 2.27759 factor:1 | -1 (0.46823) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15851 HOMO: -6.91713 LUMO: 2.28848 factor:1 | -1 (0.41549) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89927 HOMO: -7.10217 LUMO: 2.14698 factor:1 | -1 (0.67473) | 1 | 1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61201 HOMO: -6.78108 LUMO: 2.45447 factor:1 | 1 (-0.03801) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19695 HOMO: -6.78380 LUMO: 2.43542 factor:1 | 1 (-0.62295) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10391 HOMO: -6.60965 LUMO: 2.33474 factor:1 | 1 (-0.52991) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89300 HOMO: -6.72665 LUMO: 2.25855 factor:1 | 1 (-0.31900) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11420 HOMO: -6.27495 LUMO: 2.04358 factor:1 | 1 (-0.54020) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.02009 HOMO: -6.17426 LUMO: 1.45853 factor:1 | 1 (-1.44609) | -1 | -1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26278 HOMO: -7.21374 LUMO: 2.33474 factor:1 | -1 (0.31122) | 1 | 1 |
| G: -5684.20830 HOMO: -7.74164 LUMO: 1.37690 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89182 HOMO: -6.94707 LUMO: 1.81772 factor:1 | 1 (-1.31782) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.48353 HOMO: -6.80829 LUMO: 0.17960 factor:1 | 1 (-1.90953) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.02281 HOMO: -7.19469 LUMO: 1.60819 factor:1 | 1 (-1.44882) | 1 | 1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.52688 HOMO: -6.78652 LUMO: 0.53334 factor:1 | 1 (-1.95288) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.73388 HOMO: -6.70489 LUMO: 0.74559 factor:1 | 1 (-2.15988) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.03509 HOMO: -6.72393 LUMO: 0.88981 factor:1 | 1 (-1.46109) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78477 HOMO: -4.54430 LUMO: -0.90614 factor:1 | 1 (-1.21077) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.26053 HOMO: -6.83006 LUMO: 0.47348 factor:1 | 1 (-1.68653) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55720 HOMO: -7.07496 LUMO: 0.50613 factor:1 | 1 (-0.98320) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52702 HOMO: -6.62053 LUMO: 0.74559 factor:1 | 1 (-0.95302) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67650 HOMO: -6.79196 LUMO: 1.80139 factor:1 | 1 (-1.10250) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45633 HOMO: -6.71033 LUMO: 0.40817 factor:1 | 1 (-0.88233) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90257 HOMO: -6.74026 LUMO: 0.95784 factor:1 | 1 (-1.32857) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98367 HOMO: -7.34707 LUMO: 0.40001 factor:1 | 1 (-0.40967) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10187 HOMO: -6.19875 LUMO: -0.88709 factor:1 | 1 (-0.52787) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97866 HOMO: -6.48719 LUMO: -0.14694 factor:1 | 1 (-0.40466) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90897 HOMO: -6.73482 LUMO: -0.01633 factor:1 | 1 (-0.33497) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86268 HOMO: -7.05591 LUMO: -0.20136 factor:1 | 1 (-1.28868) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.03759 HOMO: -6.38651 LUMO: -2.07895 factor:1 | 1 (-1.46359) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50365 HOMO: -6.85455 LUMO: -1.03403 factor:1 | 1 (-0.92965) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49187 HOMO: -6.72121 LUMO: -0.99322 factor:1 | 1 (-0.91787) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48234 HOMO: -6.53890 LUMO: -0.10885 factor:1 | 1 (-0.90834) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.94878 HOMO: -6.68312 LUMO: 0.21225 factor:1 | -1 (2.62522) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.65026 HOMO: -6.68040 LUMO: 0.21225 factor:1 | -1 (1.92374) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55173 HOMO: -6.76475 LUMO: -0.64491 factor:1 | 1 (-0.97773) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72191 HOMO: -6.48175 LUMO: 0.41633 factor:1 | 1 (-1.14791) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52599 HOMO: -6.42733 LUMO: 0.16599 factor:1 | 1 (-0.95199) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51789 HOMO: -6.66679 LUMO: 0.77825 factor:1 | -1 (0.05611) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06051 HOMO: -6.75931 LUMO: -0.73471 factor:1 | 1 (-0.48651) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.18960 HOMO: -6.53617 LUMO: 0.38096 factor:1 | 1 (-0.61560) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29171 HOMO: -6.34297 LUMO: 0.35375 factor:1 | -1 (0.28229) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84154 HOMO: -7.11850 LUMO: -0.03265 factor:1 | 1 (-0.26754) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78646 HOMO: -5.21914 LUMO: 1.29798 factor:1 | 1 (-1.21246) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01496 HOMO: -7.09129 LUMO: -0.66668 factor:1 | 1 (-0.44096) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93256 HOMO: -6.96884 LUMO: -0.31021 factor:1 | 1 (-0.35856) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61701 HOMO: -6.51713 LUMO: -0.59865 factor:1 | 1 (-1.04301) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12182 HOMO: -6.69400 LUMO: -0.07075 factor:1 | 1 (-0.54782) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.02798 HOMO: -5.28173 LUMO: 1.17281 factor:1 | -1 (0.54602) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26232 HOMO: -6.54434 LUMO: 0.32109 factor:1 | -1 (0.31168) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.34257 HOMO: -6.79740 LUMO: -0.24762 factor:1 | -1 (0.23143) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.32398 HOMO: -6.91986 LUMO: -0.14694 factor:1 | -1 (0.25002) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51038 HOMO: -6.75114 LUMO: 0.18504 factor:1 | -1 (0.06362) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55791 HOMO: -6.74842 LUMO: 0.69389 factor:1 | 1 (-0.98391) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.22007 HOMO: -7.01782 LUMO: 0.56600 factor:1 | 1 (-1.64607) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84262 HOMO: -6.47359 LUMO: -0.56600 factor:1 | 1 (-1.26862) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10838 HOMO: -6.63686 LUMO: -0.55783 factor:1 | 1 (-0.53438) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76107 HOMO: -4.13885 LUMO: -2.05446 factor:1 | 1 (-1.18707) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74638 HOMO: -6.34570 LUMO: 0.19864 factor:1 | 1 (-0.17238) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89271 HOMO: -6.47903 LUMO: 0.24762 factor:1 | -1 (0.68129) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.88294 HOMO: -6.15249 LUMO: 0.32109 factor:1 | -1 (0.69106) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94650 HOMO: -6.84366 LUMO: 0.29116 factor:1 | -1 (0.62749) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96522 HOMO: -6.34297 LUMO: 0.19864 factor:1 | 1 (-0.39122) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03673 HOMO: -6.51168 LUMO: 0.30749 factor:1 | 1 (-0.46273) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13970 HOMO: -6.79468 LUMO: -0.16599 factor:1 | 1 (-0.56570) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50964 HOMO: -7.24095 LUMO: 0.15238 factor:1 | -1 (0.06435) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13289 HOMO: -7.06952 LUMO: -0.34558 factor:1 | 1 (-0.55889) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52434 HOMO: -6.88176 LUMO: 0.02177 factor:1 | -1 (0.04966) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12353 HOMO: -6.37291 LUMO: -0.69117 factor:1 | 1 (-0.54953) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.78122 HOMO: -6.83278 LUMO: -0.59049 factor:1 | -1 (0.79278) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.23731 HOMO: -6.57155 LUMO: -0.33470 factor:1 | -1 (0.33669) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.95663 HOMO: -6.89537 LUMO: -0.58504 factor:1 | -1 (0.61737) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.24792 HOMO: -6.57155 LUMO: -0.34831 factor:1 | -1 (0.32607) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.00340 HOMO: -6.64774 LUMO: -0.95784 factor:1 | -1 (0.57060) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86369 HOMO: -6.91713 LUMO: -0.69933 factor:1 | 1 (-0.28969) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83528 HOMO: -6.80557 LUMO: -0.65035 factor:1 | 1 (-0.26128) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99510 HOMO: -7.26544 LUMO: -0.79729 factor:1 | 1 (-0.42110) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.16596 HOMO: -6.69128 LUMO: -0.16871 factor:1 | -1 (0.40803) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08525 HOMO: -6.88448 LUMO: 0.13061 factor:1 | 1 (-0.51125) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.41547 HOMO: -6.50352 LUMO: 0.12245 factor:1 | -1 (0.15853) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.23639 HOMO: -6.56067 LUMO: 0.17687 factor:1 | -1 (0.33761) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03550 HOMO: -6.70216 LUMO: 0.25034 factor:1 | 1 (-0.46151) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.36931 HOMO: -6.51713 LUMO: -0.78369 factor:1 | -1 (0.20468) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.27584 HOMO: -6.50352 LUMO: 0.12245 factor:1 | -1 (0.29816) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83196 HOMO: -6.22052 LUMO: -0.83811 factor:1 | 1 (-0.25796) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90143 HOMO: -6.51168 LUMO: -0.76464 factor:1 | 1 (-0.32743) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28811 HOMO: -7.14571 LUMO: -0.80274 factor:1 | 1 (-0.71411) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.02248 HOMO: -6.66679 LUMO: -0.88709 factor:1 | -1 (0.55152) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.99978 HOMO: -6.76203 LUMO: -1.43948 factor:1 | -1 (0.57421) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.01671 HOMO: -6.57427 LUMO: -1.62996 factor:1 | -1 (0.55729) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05053 HOMO: -5.05043 LUMO: 1.24900 factor:1 | -1 (0.52347) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.87878 HOMO: -6.53345 LUMO: 0.23130 factor:1 | -1 (0.69522) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.22659 HOMO: -7.18381 LUMO: -0.22585 factor:1 | -1 (0.34741) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.97845 HOMO: -7.00965 LUMO: -1.79595 factor:1 | -1 (0.59555) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.93118 HOMO: -6.08174 LUMO: -0.82995 factor:1 | -1 (0.64281) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94947 HOMO: -6.42189 LUMO: -0.84355 factor:1 | -1 (0.62453) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76912 HOMO: -6.53890 LUMO: 0.60409 factor:1 | 1 (-1.19512) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94435 HOMO: -6.62869 LUMO: 0.43810 factor:1 | 1 (-0.37035) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69898 HOMO: -6.68312 LUMO: 0.64491 factor:1 | 1 (-0.12498) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03365 HOMO: -6.42189 LUMO: 1.51295 factor:1 | 1 (-0.45965) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.17448 HOMO: -6.17971 LUMO: 1.67622 factor:1 | -1 (0.39952) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.90423 HOMO: -6.79196 LUMO: 1.36873 factor:1 | -1 (1.66977) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.97302 HOMO: -7.38517 LUMO: 0.56328 factor:1 | -1 (1.60098) | 1 | 1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.71903 HOMO: -7.56204 LUMO: 0.71566 factor:1 | -1 (1.85497) | 1 | 1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13516 HOMO: -6.45726 LUMO: -1.91840 factor:1 | -1 (0.43884) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73014 HOMO: -6.13073 LUMO: -0.97417 factor:1 | 1 (-0.15614) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76989 HOMO: -6.50352 LUMO: -0.69661 factor:1 | 1 (-0.19589) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.83371 HOMO: -6.76747 LUMO: -1.71976 factor:1 | -1 (0.74029) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.92615 HOMO: -6.48447 LUMO: -0.89525 factor:1 | -1 (0.64785) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.90033 HOMO: -7.11850 LUMO: -0.71566 factor:1 | -1 (0.67367) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.68321 HOMO: -6.80285 LUMO: -0.49253 factor:1 | -1 (0.89079) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.95484 HOMO: -6.80557 LUMO: -0.88165 factor:1 | -1 (1.61916) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.32779 HOMO: -6.94162 LUMO: -0.08980 factor:1 | -1 (0.24621) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.46201 HOMO: -6.97972 LUMO: -0.29388 factor:1 | -1 (1.11199) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.05128 HOMO: -6.75114 LUMO: 0.04626 factor:1 | 1 (-1.47728) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24226 HOMO: -7.15932 LUMO: 0.68845 factor:1 | 1 (-0.66826) | 1 | 1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53007 HOMO: -7.36612 LUMO: 0.63675 factor:1 | 1 (-0.95607) | 1 | 1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.04682 HOMO: -7.02598 LUMO: -0.66124 factor:1 | 1 (-1.47282) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68077 HOMO: -6.89264 LUMO: -0.54967 factor:1 | 1 (-1.10677) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88805 HOMO: -6.97700 LUMO: 0.27756 factor:1 | 1 (-0.31405) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22669 HOMO: -6.60965 LUMO: 0.08163 factor:1 | 1 (-0.65269) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85221 HOMO: -6.70761 LUMO: 0.40001 factor:1 | 1 (-0.27821) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.31269 HOMO: -6.69128 LUMO: 0.23674 factor:1 | -1 (0.26131) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57057 HOMO: -6.69128 LUMO: -0.69933 factor:1 | -1 (0.00343) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.77412 HOMO: -6.18515 LUMO: -0.85988 factor:1 | -1 (0.79988) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19429 HOMO: -6.86815 LUMO: -1.90208 factor:1 | -1 (0.37971) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.96210 HOMO: -6.37563 LUMO: -1.74697 factor:1 | -1 (0.61190) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.76914 HOMO: -6.75659 LUMO: 0.36463 factor:1 | -1 (0.80486) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83974 HOMO: -6.91441 LUMO: -0.88981 factor:1 | 1 (-1.26574) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97949 HOMO: -6.71305 LUMO: -0.29933 factor:1 | 1 (-1.40550) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31132 HOMO: -6.91441 LUMO: -1.04492 factor:1 | 1 (-0.73732) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13608 HOMO: -6.05453 LUMO: -0.83539 factor:1 | 1 (-0.56208) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.05604 HOMO: -7.35252 LUMO: -0.45715 factor:1 | 1 (-1.48204) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19624 HOMO: -6.41644 LUMO: -0.97417 factor:1 | 1 (-0.62224) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.75138 HOMO: -6.78924 LUMO: 0.36735 factor:1 | 1 (-1.17738) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24285 HOMO: -6.74298 LUMO: 0.51974 factor:1 | 1 (-0.66886) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81811 HOMO: -6.48992 LUMO: 1.44765 factor:1 | 1 (-0.24411) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.37204 HOMO: -6.12528 LUMO: 1.57826 factor:1 | -1 (0.20196) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80472 HOMO: -6.62325 LUMO: 1.57826 factor:1 | 1 (-0.23073) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87751 HOMO: -6.19875 LUMO: 1.29798 factor:1 | 1 (-1.30351) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.13152 HOMO: -6.74570 LUMO: 1.52112 factor:1 | 1 (-1.55753) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.77537 HOMO: -6.84094 LUMO: 1.48574 factor:1 | 1 (-2.20137) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.70832 HOMO: -6.85183 LUMO: 0.33470 factor:1 | 1 (-2.13433) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97090 HOMO: -6.51168 LUMO: 0.48164 factor:1 | 1 (-1.39690) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94057 HOMO: -6.25046 LUMO: 0.75648 factor:1 | -1 (0.63343) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.96512 HOMO: -6.65591 LUMO: 0.32109 factor:1 | -1 (0.60888) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19527 HOMO: -6.71033 LUMO: 0.40817 factor:1 | -1 (0.37873) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96837 HOMO: -6.75114 LUMO: 0.73471 factor:1 | 1 (-0.39437) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29908 HOMO: -6.50624 LUMO: 0.59321 factor:1 | -1 (0.27492) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85564 HOMO: -6.39740 LUMO: 0.83267 factor:1 | 1 (-0.28164) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80053 HOMO: -6.44094 LUMO: 0.65579 factor:1 | 1 (-0.22653) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.18664 HOMO: -6.52257 LUMO: 0.05714 factor:1 | -1 (0.38735) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19777 HOMO: -7.10217 LUMO: 0.49797 factor:1 | -1 (0.37622) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98261 HOMO: -6.83006 LUMO: 0.55783 factor:1 | 1 (-0.40861) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.28520 HOMO: -6.99333 LUMO: -0.79457 factor:1 | -1 (0.28879) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02127 HOMO: -6.64230 LUMO: 0.32382 factor:1 | 1 (-0.44727) | -1 | -1 |
| G: -5684.20830 HOMO: -9.80698 LUMO: 0.51974 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43604 HOMO: -6.90897 LUMO: 0.30749 factor:1 | -1 (0.13796) | -1 | -1 |
| G: -5684.20830 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67005 HOMO: -7.09129 LUMO: 1.33336 factor:1 | 1 (-1.09605) | 1 | 1 |
| G: -5684.20830 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62812 HOMO: -6.66951 LUMO: 1.34424 factor:1 | 1 (-0.05412) | -1 | -1 |
| G: -5684.20830 HOMO: -7.26544 LUMO: -1.10478 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64668 HOMO: -7.02870 LUMO: 1.48574 factor:1 | 1 (-0.07268) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79893 HOMO: -7.26544 LUMO: 0.32926 factor:1 | 1 (-0.22493) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63634 HOMO: -6.56067 LUMO: -0.45987 factor:1 | 1 (-0.06234) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73299 HOMO: -6.54434 LUMO: -0.28300 factor:1 | 1 (-0.15900) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.75307 HOMO: -7.19469 LUMO: 0.54695 factor:1 | 1 (-1.17907) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61886 HOMO: -6.47359 LUMO: -0.22041 factor:1 | 1 (-1.04486) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.42932 HOMO: -6.80013 LUMO: 2.08167 factor:1 | -1 (0.14468) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.46670 HOMO: -6.23957 LUMO: 1.67894 factor:1 | -1 (0.10729) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.76803 HOMO: -6.75114 LUMO: -0.62858 factor:1 | 1 (-2.19403) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01207 HOMO: -6.79468 LUMO: -0.64491 factor:1 | 1 (-1.43807) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85032 HOMO: -6.84911 LUMO: -0.69661 factor:1 | 1 (-1.27632) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78020 HOMO: -7.54028 LUMO: 0.25851 factor:1 | 1 (-1.20620) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77674 HOMO: -6.92802 LUMO: -0.71022 factor:1 | 1 (-1.20274) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51282 HOMO: -6.72665 LUMO: -0.46804 factor:1 | 1 (-0.93882) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29630 HOMO: -6.63686 LUMO: -0.23674 factor:1 | 1 (-0.72230) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41869 HOMO: -7.21102 LUMO: 0.54423 factor:1 | 1 (-0.84470) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57143 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-0.99743) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47641 HOMO: -6.70761 LUMO: -0.31837 factor:1 | 1 (-0.90241) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50615 HOMO: -6.57155 LUMO: 1.76874 factor:1 | 1 (-0.93215) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.54938 HOMO: -6.84366 LUMO: 2.04358 factor:1 | -1 (1.02462) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.62221 HOMO: -6.60420 LUMO: 1.80139 factor:1 | -1 (1.95179) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.39713 HOMO: -7.03686 LUMO: 2.21229 factor:1 | -1 (1.17687) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98581 HOMO: -6.77564 LUMO: 1.97555 factor:1 | 1 (-1.41181) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30797 HOMO: -6.40012 LUMO: 2.17691 factor:1 | 1 (-0.73397) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83329 HOMO: -6.80013 LUMO: 2.25582 factor:1 | 1 (-1.25929) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33711 HOMO: -6.74298 LUMO: 2.31569 factor:1 | 1 (-0.76312) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87522 HOMO: -6.68856 LUMO: 1.85854 factor:1 | 1 (-1.30122) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67116 HOMO: -6.17971 LUMO: 1.52928 factor:1 | 1 (-1.09716) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15670 HOMO: -6.54162 LUMO: 1.91840 factor:1 | 1 (-0.58270) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59048 HOMO: -6.80013 LUMO: -0.55511 factor:1 | 1 (-1.01648) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.28244 HOMO: -7.46953 LUMO: 0.28572 factor:1 | -1 (1.29156) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.62237 HOMO: -6.61781 LUMO: -0.54967 factor:1 | -1 (1.95163) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.40811 HOMO: -6.56339 LUMO: -0.47892 factor:1 | 1 (-0.83411) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02375 HOMO: -6.65591 LUMO: -0.25307 factor:1 | 1 (-0.44975) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76262 HOMO: -6.62869 LUMO: -0.23402 factor:1 | 1 (-1.18862) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10538 HOMO: -6.58243 LUMO: -0.19048 factor:1 | 1 (-0.53138) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.88608 HOMO: -7.27632 LUMO: 0.52790 factor:1 | 1 (-1.31208) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14168 HOMO: -7.21102 LUMO: 0.57688 factor:1 | 1 (-0.56768) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.12180 HOMO: -6.72393 LUMO: -0.53879 factor:1 | -1 (0.45220) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.05011 HOMO: -7.42054 LUMO: -0.99322 factor:1 | -1 (1.52389) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.00107 HOMO: -6.88992 LUMO: -0.71838 factor:1 | -1 (1.57293) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.42481 HOMO: -6.88176 LUMO: -0.61226 factor:1 | -1 (1.14919) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.09686 HOMO: -7.36340 LUMO: -1.04492 factor:1 | -1 (2.47713) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.95471 HOMO: -6.65863 LUMO: -0.41906 factor:1 | -1 (2.61929) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.11225 HOMO: -7.15115 LUMO: -0.66396 factor:1 | -1 (0.46175) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.07598 HOMO: -7.10489 LUMO: -0.64491 factor:1 | -1 (1.49801) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.31606 HOMO: -7.20285 LUMO: 0.47892 factor:1 | -1 (0.25794) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.53722 HOMO: -6.55794 LUMO: -0.28844 factor:1 | -1 (1.03678) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.97626 HOMO: -7.19197 LUMO: -0.69661 factor:1 | -1 (1.59774) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70105 HOMO: -6.56883 LUMO: -0.32926 factor:1 | 1 (-0.12705) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.15797 HOMO: -6.70761 LUMO: 1.95650 factor:1 | 1 (-1.58397) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.25986 HOMO: -6.60420 LUMO: 1.80684 factor:1 | 1 (-0.68586) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.11999 HOMO: -6.84094 LUMO: 1.64085 factor:1 | 1 (-1.54599) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24500 HOMO: -6.69128 LUMO: 1.90208 factor:1 | 1 (-0.67101) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87353 HOMO: -6.75387 LUMO: 1.70343 factor:1 | 1 (-1.29953) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14925 HOMO: -7.07496 LUMO: 2.10072 factor:1 | 1 (-0.57525) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74113 HOMO: -6.99877 LUMO: 2.24494 factor:1 | 1 (-0.16713) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.50378 HOMO: -6.63414 LUMO: 2.17691 factor:1 | -1 (1.07022) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.17909 HOMO: -6.44638 LUMO: 1.78235 factor:1 | -1 (1.39491) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.12806 HOMO: -6.87632 LUMO: 1.84221 factor:1 | -1 (0.44594) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85419 HOMO: -6.85183 LUMO: 1.68711 factor:1 | 1 (-0.28020) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79560 HOMO: -6.96339 LUMO: 2.26671 factor:1 | 1 (-1.22160) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02500 HOMO: -6.63141 LUMO: 1.96738 factor:1 | 1 (-0.45100) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.56575 HOMO: -6.37019 LUMO: 2.23133 factor:1 | 1 (-0.99175) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.07699 HOMO: -7.11034 LUMO: 2.32385 factor:1 | 1 (-1.50299) | 1 | 1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28778 HOMO: -6.91986 LUMO: 1.65445 factor:1 | 1 (-0.71378) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12133 HOMO: -7.12938 LUMO: 2.28304 factor:1 | 1 (-0.54733) | 1 | 1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94146 HOMO: -6.54978 LUMO: 1.92112 factor:1 | 1 (-0.36746) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.21196 HOMO: -6.83006 LUMO: 2.48712 factor:1 | -1 (1.36204) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05535 HOMO: -6.97972 LUMO: 1.96738 factor:1 | -1 (0.51865) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.37059 HOMO: -6.69944 LUMO: 2.06262 factor:1 | -1 (0.20341) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.52908 HOMO: -6.76747 LUMO: 2.10888 factor:1 | -1 (1.04492) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70211 HOMO: -6.91169 LUMO: 2.06534 factor:1 | 1 (-0.12811) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.95454 HOMO: -7.03414 LUMO: 1.93473 factor:1 | 1 (-1.38054) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31608 HOMO: -7.03142 LUMO: 2.52250 factor:1 | 1 (-0.74208) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10555 HOMO: -6.34025 LUMO: 2.61229 factor:1 | 1 (-0.53155) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00458 HOMO: -6.98788 LUMO: 2.28304 factor:1 | 1 (-1.43058) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.96417 HOMO: -6.97700 LUMO: 2.53882 factor:1 | 1 (-1.39018) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24672 HOMO: -6.58788 LUMO: 1.94289 factor:1 | 1 (-0.67272) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.10023 HOMO: -6.78652 LUMO: 2.13609 factor:1 | 1 (-1.52623) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.40852 HOMO: -6.55250 LUMO: 1.82861 factor:1 | 1 (-0.83452) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80534 HOMO: -6.45998 LUMO: 1.75786 factor:1 | 1 (-1.23134) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.85679 HOMO: -6.78924 LUMO: 2.33746 factor:1 | -1 (0.71721) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63618 HOMO: -6.85727 LUMO: 1.76058 factor:1 | 1 (-0.06218) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.04581 HOMO: -6.70489 LUMO: 1.84493 factor:1 | -1 (1.52819) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.68454 HOMO: -6.71305 LUMO: 1.53472 factor:1 | -1 (0.88946) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.93766 HOMO: -6.76747 LUMO: 1.48846 factor:1 | -1 (0.63634) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89528 HOMO: -6.69128 LUMO: 1.95922 factor:1 | 1 (-0.32128) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.46623 HOMO: -6.67495 LUMO: 2.05446 factor:1 | 1 (-0.89223) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.32674 HOMO: -6.63686 LUMO: 2.25310 factor:1 | 1 (-1.75274) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24119 HOMO: -6.63958 LUMO: 2.14154 factor:1 | 1 (-0.66720) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94279 HOMO: -6.62597 LUMO: 2.01908 factor:1 | 1 (-1.36879) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91964 HOMO: -7.07768 LUMO: 2.14154 factor:1 | 1 (-0.34564) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.76441 HOMO: -6.19603 LUMO: 2.01092 factor:1 | -1 (1.80958) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.58774 HOMO: -6.65046 LUMO: 2.15786 factor:1 | 1 (-0.01374) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.71417 HOMO: -6.92258 LUMO: 2.31841 factor:1 | -1 (0.85983) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77253 HOMO: -6.90081 LUMO: 2.19324 factor:1 | 1 (-0.19853) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.86016 HOMO: -6.85455 LUMO: 1.95650 factor:1 | -1 (0.71384) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87863 HOMO: -6.57699 LUMO: 1.76058 factor:1 | 1 (-0.30463) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63035 HOMO: -6.90625 LUMO: 1.97555 factor:1 | 1 (-0.05635) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.34866 HOMO: -6.97428 LUMO: 1.92929 factor:1 | -1 (0.22534) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07654 HOMO: -6.61781 LUMO: -0.41906 factor:1 | 1 (-0.50254) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98975 HOMO: -6.62869 LUMO: -0.81906 factor:1 | 1 (-1.41575) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07967 HOMO: -7.01237 LUMO: 2.00548 factor:1 | 1 (-0.50567) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50871 HOMO: -6.85727 LUMO: 2.17691 factor:1 | 1 (-0.93471) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01088 HOMO: -6.71849 LUMO: 1.58914 factor:1 | 1 (-0.43688) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51938 HOMO: -7.52395 LUMO: 0.27211 factor:1 | 1 (-0.94538) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02111 HOMO: -6.96611 LUMO: -0.72654 factor:1 | 1 (-0.44711) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76791 HOMO: -6.89537 LUMO: -0.68028 factor:1 | 1 (-0.19391) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99224 HOMO: -6.84911 LUMO: -0.58504 factor:1 | 1 (-0.41824) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89732 HOMO: -6.79196 LUMO: -0.55783 factor:1 | 1 (-0.32333) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85446 HOMO: -6.67767 LUMO: 1.79323 factor:1 | 1 (-1.28046) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26880 HOMO: -6.54434 LUMO: 1.91024 factor:1 | -1 (0.30520) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13619 HOMO: -6.62869 LUMO: 1.69799 factor:1 | -1 (0.43780) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79362 HOMO: -6.72393 LUMO: 2.12249 factor:1 | 1 (-0.21962) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66937 HOMO: -6.66407 LUMO: 2.05990 factor:1 | 1 (-0.09538) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.40797 HOMO: -7.00149 LUMO: 1.82044 factor:1 | 1 (-0.83397) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92535 HOMO: -7.12122 LUMO: 2.16058 factor:1 | 1 (-0.35135) | 1 | 1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94120 HOMO: -6.63141 LUMO: 2.21229 factor:1 | -1 (0.63280) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64342 HOMO: -6.37835 LUMO: 2.32113 factor:1 | 1 (-0.06942) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75000 HOMO: -6.99605 LUMO: 2.00548 factor:1 | 1 (-0.17600) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89687 HOMO: -6.85999 LUMO: 2.39460 factor:1 | -1 (0.67713) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.55341 HOMO: -6.85727 LUMO: 2.48712 factor:1 | -1 (1.02059) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.34579 HOMO: -7.04231 LUMO: 2.40277 factor:1 | -1 (2.22820) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.71854 HOMO: -6.60692 LUMO: 2.26671 factor:1 | -1 (1.85546) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.74670 HOMO: -6.67495 LUMO: 2.14698 factor:1 | -1 (1.82730) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.73350 HOMO: -6.73210 LUMO: 2.06807 factor:1 | -1 (1.84050) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.01037 HOMO: -7.20013 LUMO: 2.02181 factor:1 | -1 (0.56363) | 1 | 1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.99812 HOMO: -7.18653 LUMO: 2.29936 factor:1 | -1 (0.57587) | 1 | 1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.60753 HOMO: -6.92802 LUMO: 2.36195 factor:1 | -1 (0.96647) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64211 HOMO: -6.89537 LUMO: 1.78779 factor:1 | 1 (-0.06811) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54208 HOMO: -6.96067 LUMO: 2.31297 factor:1 | -1 (0.03192) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48716 HOMO: -6.91441 LUMO: 2.50345 factor:1 | 1 (-0.91316) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.05653 HOMO: -7.17292 LUMO: 2.12521 factor:1 | 1 (-1.48253) | 1 | 1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65942 HOMO: -6.93618 LUMO: 2.35106 factor:1 | 1 (-0.08542) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04778 HOMO: -6.75931 LUMO: 1.61908 factor:1 | 1 (-0.47378) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30288 HOMO: -6.35930 LUMO: 1.23540 factor:1 | 1 (-0.72888) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.02997 HOMO: -6.17971 LUMO: 1.84493 factor:1 | 1 (-1.45597) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39222 HOMO: -6.72665 LUMO: 2.61229 factor:1 | 1 (-0.81822) | -1 | -1 |
| G: -5684.20830 HOMO: -7.09945 LUMO: 1.66806 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00834 HOMO: -6.62869 LUMO: 2.28304 factor:1 | 1 (-1.43434) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06810 HOMO: -6.58243 LUMO: 0.28028 factor:1 | 1 (-0.49410) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63905 HOMO: -6.79468 LUMO: 0.14966 factor:1 | 1 (-1.06505) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00933 HOMO: -6.63141 LUMO: 0.31021 factor:1 | 1 (-0.43533) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69410 HOMO: -6.81101 LUMO: 0.13878 factor:1 | 1 (-1.12010) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78708 HOMO: -6.72665 LUMO: 0.65579 factor:1 | 1 (-1.21308) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96470 HOMO: -6.53073 LUMO: 0.91430 factor:1 | 1 (-0.39070) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64741 HOMO: -7.19197 LUMO: 1.62996 factor:1 | 1 (-1.07341) | 1 | 1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47671 HOMO: -6.69400 LUMO: 0.84627 factor:1 | 1 (-0.90271) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.79877 HOMO: -6.76475 LUMO: 0.51974 factor:1 | -1 (0.77523) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.93026 HOMO: -6.67767 LUMO: 0.52246 factor:1 | -1 (0.64374) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15568 HOMO: -6.73210 LUMO: 0.94424 factor:1 | -1 (0.41832) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.68311 HOMO: -6.97972 LUMO: 0.60409 factor:1 | -1 (1.89089) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.64243 HOMO: -7.38517 LUMO: 0.73743 factor:1 | -1 (1.93157) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47498 HOMO: -6.48992 LUMO: 1.08301 factor:1 | -1 (0.09902) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.41756 HOMO: -7.18381 LUMO: 1.61908 factor:1 | -1 (0.15644) | 1 | 1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93248 HOMO: -6.74842 LUMO: 0.57960 factor:1 | 1 (-0.35848) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94384 HOMO: -6.67495 LUMO: 0.77280 factor:1 | -1 (0.63016) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87702 HOMO: -6.74570 LUMO: 0.77280 factor:1 | 1 (-0.30303) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.97616 HOMO: -6.73754 LUMO: 0.86804 factor:1 | -1 (0.59783) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57707 HOMO: -6.66135 LUMO: 0.94424 factor:1 | 1 (-0.00307) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52164 HOMO: -6.44638 LUMO: 1.00138 factor:1 | -1 (0.05235) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48638 HOMO: -6.65591 LUMO: 1.02043 factor:1 | -1 (0.08762) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07355 HOMO: -7.17564 LUMO: 0.50069 factor:1 | 1 (-0.49955) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01174 HOMO: -6.59332 LUMO: 0.79457 factor:1 | 1 (-1.43774) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63151 HOMO: -6.76747 LUMO: 1.73881 factor:1 | 1 (-1.05752) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06491 HOMO: -7.00421 LUMO: 1.07485 factor:1 | 1 (-1.49091) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13110 HOMO: -6.94979 LUMO: 1.67894 factor:1 | 1 (-0.55710) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.09898 HOMO: -6.66135 LUMO: 0.47076 factor:1 | 1 (-1.52498) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41616 HOMO: -6.74298 LUMO: 1.85037 factor:1 | 1 (-0.84217) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65620 HOMO: -6.65318 LUMO: 0.95240 factor:1 | 1 (-0.08221) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55657 HOMO: -6.63958 LUMO: 0.78097 factor:1 | 1 (-0.98258) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67927 HOMO: -6.11712 LUMO: 0.40001 factor:1 | 1 (-1.10527) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04408 HOMO: -7.08312 LUMO: 0.92519 factor:1 | 1 (-0.47008) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90380 HOMO: -6.96067 LUMO: 0.54695 factor:1 | 1 (-0.32980) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.56032 HOMO: -6.74026 LUMO: 0.60137 factor:1 | -1 (1.01368) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.53365 HOMO: -6.74298 LUMO: 0.59593 factor:1 | -1 (1.04035) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68050 HOMO: -6.93074 LUMO: 0.60681 factor:1 | 1 (-0.10651) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80521 HOMO: -6.41644 LUMO: 0.35919 factor:1 | 1 (-0.23122) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57931 HOMO: -6.41917 LUMO: 1.73064 factor:1 | 1 (-0.00531) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53422 HOMO: -4.64226 LUMO: -0.87893 factor:1 | -1 (0.03978) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97624 HOMO: -6.59604 LUMO: 0.90342 factor:1 | 1 (-0.40224) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33091 HOMO: -6.79468 LUMO: 0.50069 factor:1 | 1 (-0.75691) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51285 HOMO: -7.04503 LUMO: 0.52518 factor:1 | 1 (-0.93885) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84829 HOMO: -6.69400 LUMO: 0.54423 factor:1 | 1 (-0.27429) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83272 HOMO: -6.51713 LUMO: 0.95240 factor:1 | 1 (-1.25872) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08710 HOMO: -6.88176 LUMO: 1.79323 factor:1 | 1 (-0.51310) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05521 HOMO: -6.71849 LUMO: 0.28844 factor:1 | 1 (-0.48121) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52166 HOMO: -6.94979 LUMO: 0.51974 factor:1 | 1 (-0.94766) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97759 HOMO: -6.76203 LUMO: 0.94151 factor:1 | 1 (-1.40359) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06546 HOMO: -6.91169 LUMO: 0.89525 factor:1 | 1 (-0.49146) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03463 HOMO: -6.83006 LUMO: 0.89253 factor:1 | 1 (-0.46063) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05627 HOMO: -7.08857 LUMO: 0.60409 factor:1 | 1 (-0.48227) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48249 HOMO: -6.91713 LUMO: 1.76330 factor:1 | -1 (0.09151) | -1 | -1 |
| G: -5684.20830 HOMO: -8.88180 LUMO: 1.02315 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.53059 HOMO: -6.47359 LUMO: 1.56193 factor:1 | -1 (2.04341) | -1 | -1 |
| G: -5684.20830 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.88559 HOMO: -7.00149 LUMO: 1.47214 factor:1 | -1 (1.68841) | -1 | -1 |
| G: -5684.20830 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.39644 HOMO: -7.03686 LUMO: 1.97283 factor:1 | -1 (0.17755) | -1 | -1 |
| G: -5684.20830 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.21354 HOMO: -7.00965 LUMO: 1.64629 factor:1 | -1 (1.36046) | -1 | -1 |
| G: -5684.20830 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.45411 HOMO: -7.06952 LUMO: 1.67622 factor:1 | -1 (1.11988) | 1 | -1 |
| G: -5684.20830 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.17237 HOMO: -6.80557 LUMO: 1.70615 factor:1 | -1 (1.40163) | -1 | -1 |
| G: -5684.20830 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.17849 HOMO: -6.80829 LUMO: 1.71704 factor:1 | -1 (1.39551) | -1 | -1 |
| G: -5684.20830 HOMO: -6.91169 LUMO: -0.53879 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.90591 HOMO: -7.26544 LUMO: 1.89935 factor:1 | -1 (1.66809) | 1 | -1 |
| G: -5684.20830 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.08023 HOMO: -7.00149 LUMO: 1.47214 factor:1 | -1 (1.49377) | -1 | -1 |
| G: -5684.20830 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.51586 HOMO: -7.03686 LUMO: 1.97283 factor:1 | -1 (1.05814) | -1 | -1 |
| G: -5684.20830 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.72387 HOMO: -7.00965 LUMO: 1.64629 factor:1 | -1 (1.85013) | -1 | -1 |
| G: -5684.20830 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.76243 HOMO: -7.06952 LUMO: 1.67622 factor:1 | -1 (1.81157) | -1 | -1 |
| G: -5684.20830 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.07584 HOMO: -6.80557 LUMO: 1.70615 factor:1 | -1 (0.49816) | -1 | -1 |
| G: -5684.20830 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.37465 HOMO: -6.80829 LUMO: 1.71704 factor:1 | -1 (0.19935) | -1 | -1 |
| G: -5684.20830 HOMO: -7.29809 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29691 HOMO: -7.26544 LUMO: 1.89935 factor:1 | -1 (0.27709) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.11690 HOMO: -7.00149 LUMO: 1.75241 factor:1 | -1 (0.45710) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81067 HOMO: -6.91169 LUMO: 2.07079 factor:1 | -1 (0.76333) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.51297 HOMO: -7.11034 LUMO: 1.76330 factor:1 | -1 (1.06103) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.38083 HOMO: -6.87360 LUMO: 2.02725 factor:1 | -1 (1.19316) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.67420 HOMO: -7.08584 LUMO: 1.82044 factor:1 | -1 (0.89980) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.16181 HOMO: -6.90625 LUMO: 1.68166 factor:1 | -1 (1.41219) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92668 HOMO: -6.71577 LUMO: 1.93201 factor:1 | 1 (-1.35268) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99005 HOMO: -6.99605 LUMO: 2.08439 factor:1 | 1 (-1.41605) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.26184 HOMO: -7.02326 LUMO: 1.97010 factor:1 | 1 (-1.68784) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57500 HOMO: -6.99877 LUMO: 2.15514 factor:1 | 1 (-1.00100) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08820 HOMO: -6.75387 LUMO: 1.95106 factor:1 | 1 (-1.51420) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.23220 HOMO: -7.10761 LUMO: 2.06262 factor:1 | -1 (0.34180) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.30270 HOMO: -7.03142 LUMO: 1.91568 factor:1 | -1 (0.27130) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.08003 HOMO: -6.98788 LUMO: 1.98371 factor:1 | -1 (0.49397) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84643 HOMO: -6.94707 LUMO: 1.68438 factor:1 | 1 (-1.27243) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72354 HOMO: -6.88176 LUMO: 2.20684 factor:1 | 1 (-1.14955) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12628 HOMO: -6.73210 LUMO: 2.18780 factor:1 | 1 (-0.55228) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05893 HOMO: -6.83822 LUMO: 2.06807 factor:1 | 1 (-0.48493) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.32876 HOMO: -6.78924 LUMO: 2.42181 factor:1 | 1 (-0.75476) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.12227 HOMO: -6.94707 LUMO: 1.71704 factor:1 | 1 (-1.54827) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.18875 HOMO: -6.85183 LUMO: 1.78779 factor:1 | 1 (-1.61475) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60158 HOMO: -6.98788 LUMO: 1.69799 factor:1 | 1 (-1.02758) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93889 HOMO: -6.79468 LUMO: 2.04358 factor:1 | 1 (-1.36490) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78180 HOMO: -6.90081 LUMO: 1.97283 factor:1 | 1 (-1.20780) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.45382 HOMO: -6.79468 LUMO: 2.00820 factor:1 | 1 (-1.87982) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87459 HOMO: -7.06408 LUMO: 2.29936 factor:1 | 1 (-1.30060) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35537 HOMO: -6.78924 LUMO: 2.13337 factor:1 | 1 (-0.78137) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51102 HOMO: -6.79468 LUMO: 2.35106 factor:1 | 1 (-0.93702) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86394 HOMO: -6.82734 LUMO: 2.16603 factor:1 | 1 (-0.28994) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39358 HOMO: -6.79740 LUMO: 2.36739 factor:1 | 1 (-0.81958) | -1 | -1 |
| G: -5684.20830 HOMO: -7.85865 LUMO: 2.83543 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36294 HOMO: -7.14027 LUMO: 2.10888 factor:1 | 1 (-0.78894) | -1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65718 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-0.08319) | -1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21834 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.64434) | -1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48534 HOMO: -6.94707 LUMO: 1.73064 factor:1 | -1 (0.08865) | -1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.28274 HOMO: -7.02326 LUMO: 1.41227 factor:1 | -1 (1.29126) | -1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.43213 HOMO: -6.72121 LUMO: 1.43132 factor:1 | -1 (1.14187) | -1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89614 HOMO: -6.51168 LUMO: 1.72520 factor:1 | -1 (0.67786) | -1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05410 HOMO: -6.98516 LUMO: 1.92929 factor:1 | -1 (0.51990) | -1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.00836 HOMO: -6.92802 LUMO: 2.07895 factor:1 | -1 (0.56564) | -1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13894 HOMO: -7.02326 LUMO: 1.86398 factor:1 | -1 (0.43506) | -1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.20955 HOMO: -6.82462 LUMO: 1.86670 factor:1 | -1 (2.36445) | -1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.03198 HOMO: -6.83278 LUMO: 1.71160 factor:1 | -1 (1.54201) | -1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57092 HOMO: -6.62869 LUMO: 1.69527 factor:1 | -1 (0.00307) | -1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77300 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-0.19900) | -1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94537 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.37137) | 1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93174 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.35774) | 1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85602 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-0.28202) | -1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50017 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.92617) | 1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19624 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.62224) | -1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93382 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.35982) | 1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81558 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-0.24158) | -1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64381 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-1.06982) | -1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15670 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-0.58270) | -1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90170 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-1.32770) | -1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98334 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.40934) | -1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76592 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.19192) | -1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.92152 HOMO: -6.93618 LUMO: 2.19324 factor:1 | -1 (0.65247) | -1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.96041 HOMO: -6.95523 LUMO: 1.80684 factor:1 | -1 (0.61359) | -1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80021 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-0.22621) | -1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.03351 HOMO: -6.36202 LUMO: 1.89391 factor:1 | -1 (1.54049) | -1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.60076 HOMO: -7.03959 LUMO: 2.06262 factor:1 | -1 (0.97324) | -1 | -1 |
| G: -5684.20830 HOMO: -6.61509 LUMO: -0.23674 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.73660 HOMO: -7.08584 LUMO: 2.01092 factor:1 | -1 (0.83740) | 1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.53363 HOMO: -6.96067 LUMO: 1.59731 factor:1 | -1 (2.04036) | -1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.28781 HOMO: -6.91169 LUMO: 1.37145 factor:1 | -1 (2.28619) | -1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50671 HOMO: -6.94707 LUMO: 1.73064 factor:1 | -1 (0.06729) | -1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.57175 HOMO: -7.02326 LUMO: 1.41227 factor:1 | -1 (1.00225) | -1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61503 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-0.04103) | -1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.62878 HOMO: -6.51168 LUMO: 1.72520 factor:1 | -1 (0.94521) | -1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76116 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.18716) | -1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.86384 HOMO: -6.92802 LUMO: 2.07895 factor:1 | -1 (0.71016) | -1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84225 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.26825) | -1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91055 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.33655) | -1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30245 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.72845) | -1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.02701 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.45301) | -1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80624 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.23224) | -1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.49953 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-1.92553) | 1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65886 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.08486) | 1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.43518 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-1.86118) | -1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89187 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.31787) | 1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31401 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.74001) | -1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97811 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.40411) | 1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.02989 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.45589) | -1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30726 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-0.73327) | -1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.80364 HOMO: -6.98516 LUMO: 1.64629 factor:1 | -1 (0.77035) | -1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.66304 HOMO: -6.80285 LUMO: 1.95106 factor:1 | -1 (0.91096) | -1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.05212 HOMO: -6.76747 LUMO: 1.88303 factor:1 | -1 (1.52188) | -1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66837 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.09437) | -1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.90359 HOMO: -6.93618 LUMO: 2.19324 factor:1 | -1 (0.67041) | -1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.95274 HOMO: -6.95523 LUMO: 1.80684 factor:1 | -1 (0.62126) | -1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.00231 HOMO: -6.66135 LUMO: 1.72792 factor:1 | -1 (0.57168) | -1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88742 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.31342) | -1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91090 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.33690) | -1 | -1 |
| G: -5684.20830 HOMO: -6.80285 LUMO: -0.55783 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91305 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.33905) | 1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86564 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.29164) | -1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12332 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.54932) | -1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59976 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.02576) | -1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84995 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-0.27595) | -1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81467 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.24068) | -1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08604 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-0.51204) | -1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91338 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-0.33938) | -1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99977 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.42577) | -1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.27711 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-0.70312) | -1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04040 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.46640) | -1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88595 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-0.31195) | -1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.15990 HOMO: -6.62869 LUMO: 1.69527 factor:1 | -1 (1.41409) | -1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.39346 HOMO: -6.84094 LUMO: 1.27349 factor:1 | -1 (1.18054) | -1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.36519 HOMO: -7.07768 LUMO: 1.27621 factor:1 | -1 (1.20881) | -1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.31269 HOMO: -7.06135 LUMO: 1.55105 factor:1 | -1 (0.26131) | -1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.26383 HOMO: -6.94162 LUMO: 1.64629 factor:1 | -1 (2.31017) | -1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35924 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.78524) | -1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.46055 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-0.88655) | -1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.58734 HOMO: -7.09129 LUMO: 1.73609 factor:1 | -1 (0.98666) | -1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.47798 HOMO: -7.01237 LUMO: 2.01092 factor:1 | -1 (1.09602) | -1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.34576 HOMO: -6.93618 LUMO: 1.63540 factor:1 | -1 (1.22824) | -1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.40747 HOMO: -6.98516 LUMO: 1.64629 factor:1 | -1 (1.16652) | -1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08454 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.51054) | -1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73089 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-1.15689) | -1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08739 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-1.51339) | -1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85329 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.27929) | -1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24941 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.67541) | -1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97247 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-1.39847) | -1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93917 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-1.36517) | -1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.34648 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.77248) | -1 | -1 |
| G: -5684.20830 HOMO: -7.16476 LUMO: 2.86264 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92978 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-1.35578) | -1 | -1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06129 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.48729) | 1 | 1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49279 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.91879) | -1 | -1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97076 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.39676) | 1 | 1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69035 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-1.11635) | -1 | -1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.07536 HOMO: -6.72121 LUMO: 1.43132 factor:1 | -1 (1.49864) | -1 | -1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.20921 HOMO: -6.51168 LUMO: 1.72520 factor:1 | -1 (1.36479) | 1 | 1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.72041 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-2.14641) | 1 | 1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01862 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.44463) | 1 | 1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.82805 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-2.25406) | 1 | 1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00913 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-1.43513) | 1 | 1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66205 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-1.08805) | 1 | 1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69454 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.12054) | 1 | 1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.49156 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-1.91756) | -1 | -1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.94659 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-2.37259) | -1 | -1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.39384 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-1.81984) | -1 | -1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39475 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-0.82075) | 1 | 1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76727 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-1.19327) | 1 | 1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61505 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-1.04105) | 1 | 1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60888 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-1.03488) | 1 | 1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.26557 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.69157) | 1 | 1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.50720 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-1.93321) | 1 | 1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.09824 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-2.52424) | 1 | 1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.16791 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-1.59391) | 1 | 1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04125 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-0.46725) | 1 | 1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33546 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-0.76146) | 1 | 1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.04556 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.47156) | 1 | 1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99438 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-1.42038) | 1 | 1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09466 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-0.52066) | 1 | 1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10402 HOMO: -6.36202 LUMO: 1.89391 factor:1 | 1 (-0.53002) | -1 | -1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05940 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.48540) | 1 | 1 |
| G: -5684.20830 HOMO: -6.50352 LUMO: 2.10888 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73836 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.16436) | 1 | 1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91364 HOMO: -6.96067 LUMO: 1.59731 factor:1 | 1 (-1.33964) | 1 | 1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04084 HOMO: -6.91169 LUMO: 1.37145 factor:1 | 1 (-0.46684) | -1 | -1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.21680 HOMO: -6.94707 LUMO: 1.73064 factor:1 | 1 (-1.64281) | 1 | 1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93027 HOMO: -7.02326 LUMO: 1.41227 factor:1 | 1 (-1.35627) | -1 | -1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.42459 HOMO: -6.72121 LUMO: 1.43132 factor:1 | 1 (-1.85059) | -1 | -1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97759 HOMO: -6.51168 LUMO: 1.72520 factor:1 | 1 (-1.40359) | -1 | -1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.51126 HOMO: -6.98516 LUMO: 1.92929 factor:1 | 1 (-1.93726) | 1 | 1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91092 HOMO: -6.92802 LUMO: 2.07895 factor:1 | 1 (-1.33692) | 1 | 1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.19123 HOMO: -7.02326 LUMO: 1.86398 factor:1 | 1 (-1.61723) | 1 | 1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05006 HOMO: -6.82462 LUMO: 1.86670 factor:1 | 1 (-0.47606) | 1 | 1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87253 HOMO: -6.83278 LUMO: 1.71160 factor:1 | 1 (-1.29853) | 1 | 1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.07574 HOMO: -6.62869 LUMO: 1.69527 factor:1 | 1 (-1.50174) | 1 | 1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02410 HOMO: -6.84094 LUMO: 1.27349 factor:1 | 1 (-0.45010) | -1 | -1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96990 HOMO: -7.07768 LUMO: 1.27621 factor:1 | 1 (-0.39590) | -1 | -1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12881 HOMO: -7.06135 LUMO: 1.55105 factor:1 | 1 (-0.55481) | -1 | -1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61993 HOMO: -6.94162 LUMO: 1.64629 factor:1 | 1 (-0.04593) | 1 | 1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00772 HOMO: -7.07224 LUMO: 1.65445 factor:1 | 1 (-0.43372) | 1 | 1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.22500 HOMO: -6.68584 LUMO: 1.91296 factor:1 | 1 (-1.65100) | 1 | 1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05120 HOMO: -7.09129 LUMO: 1.73609 factor:1 | 1 (-0.47721) | 1 | 1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.20695 HOMO: -7.01237 LUMO: 2.01092 factor:1 | 1 (-1.63296) | 1 | 1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.75535 HOMO: -6.93618 LUMO: 1.63540 factor:1 | 1 (-1.18136) | 1 | 1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.95264 HOMO: -6.98516 LUMO: 1.64629 factor:1 | 1 (-1.37864) | 1 | 1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.34607 HOMO: -6.80285 LUMO: 1.95106 factor:1 | 1 (-0.77207) | 1 | 1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.55433 HOMO: -6.76747 LUMO: 1.88303 factor:1 | 1 (-1.98034) | 1 | 1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01571 HOMO: -6.64230 LUMO: 1.90480 factor:1 | 1 (-1.44171) | 1 | 1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.42443 HOMO: -6.93618 LUMO: 2.19324 factor:1 | 1 (-1.85043) | 1 | 1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.32566 HOMO: -6.95523 LUMO: 1.80684 factor:1 | 1 (-0.75166) | 1 | 1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17144 HOMO: -6.66135 LUMO: 1.72792 factor:1 | 1 (-1.59744) | 1 | 1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.24782 HOMO: -6.36202 LUMO: 1.89391 factor:1 | -1 (0.32618) | -1 | -1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94832 HOMO: -7.03959 LUMO: 2.06262 factor:1 | 1 (-0.37432) | 1 | 1 |
| G: -5684.20830 HOMO: -6.59604 LUMO: 2.33746 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60586 HOMO: -7.08584 LUMO: 2.01092 factor:1 | 1 (-0.03186) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81659 HOMO: -7.06135 LUMO: 0.75376 factor:1 | 1 (-0.24259) | 1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71713 HOMO: -5.10213 LUMO: 0.77825 factor:1 | 1 (-0.14313) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.17590 HOMO: -5.84228 LUMO: 0.50341 factor:1 | -1 (0.39810) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91041 HOMO: -5.39874 LUMO: 0.68028 factor:1 | 1 (-0.33641) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.50927 HOMO: -5.16744 LUMO: 1.14832 factor:1 | 1 (-1.93527) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51143 HOMO: -5.80963 LUMO: 0.35647 factor:1 | 1 (-0.93743) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08728 HOMO: -5.02322 LUMO: 1.07213 factor:1 | 1 (-1.51328) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.09465 HOMO: -5.80963 LUMO: 0.56328 factor:1 | 1 (-1.52065) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48175 HOMO: -5.45316 LUMO: 0.78369 factor:1 | -1 (0.09225) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06418 HOMO: -5.25452 LUMO: 0.82178 factor:1 | 1 (-0.49019) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01003 HOMO: -5.21370 LUMO: 1.03947 factor:1 | 1 (-0.43604) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30452 HOMO: -6.04365 LUMO: 0.31837 factor:1 | 1 (-0.73052) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68268 HOMO: -5.86405 LUMO: 0.55511 factor:1 | 1 (-0.10868) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21616 HOMO: -5.64908 LUMO: 0.71022 factor:1 | 1 (-0.64216) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85375 HOMO: -5.94297 LUMO: 0.68301 factor:1 | 1 (-1.27975) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12247 HOMO: -6.01916 LUMO: 0.56328 factor:1 | 1 (-0.54847) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68575 HOMO: -6.05181 LUMO: 0.35103 factor:1 | 1 (-1.11175) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95839 HOMO: -6.08447 LUMO: 0.48436 factor:1 | 1 (-0.38439) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.18960 HOMO: -5.86950 LUMO: 0.36735 factor:1 | 1 (-0.61560) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05504 HOMO: -5.33615 LUMO: 0.65852 factor:1 | 1 (-0.48104) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81574 HOMO: -5.36064 LUMO: 0.86804 factor:1 | 1 (-1.24174) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.04872 HOMO: -5.74160 LUMO: 0.64491 factor:1 | 1 (-1.47472) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01461 HOMO: -5.23003 LUMO: 0.66124 factor:1 | 1 (-0.44061) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76953 HOMO: -5.77698 LUMO: 0.84083 factor:1 | 1 (-1.19553) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.56596 HOMO: -5.60555 LUMO: 0.84355 factor:1 | 1 (-0.99196) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.96194 HOMO: -7.11578 LUMO: -1.62452 factor:1 | 1 (-1.38794) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55116 HOMO: -7.23279 LUMO: -1.63813 factor:1 | 1 (-0.97716) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09583 HOMO: -6.68312 LUMO: -0.88709 factor:1 | 1 (-0.52183) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06541 HOMO: -6.99333 LUMO: -0.88709 factor:1 | 1 (-0.49141) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93588 HOMO: -7.40694 LUMO: 0.11973 factor:1 | 1 (-0.36188) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80330 HOMO: -6.74026 LUMO: -0.72927 factor:1 | 1 (-1.22930) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.39885 HOMO: -6.67223 LUMO: -0.70750 factor:1 | 1 (-1.82485) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59568 HOMO: -7.06952 LUMO: -1.40139 factor:1 | 1 (-1.02168) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08657 HOMO: -7.21374 LUMO: -1.13199 factor:1 | 1 (-1.51257) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.49014 HOMO: -6.54706 LUMO: -1.34424 factor:1 | 1 (-1.91614) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.16799 HOMO: -7.51851 LUMO: -1.05852 factor:1 | 1 (-1.59399) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.94036 HOMO: -7.07224 LUMO: -1.89391 factor:1 | 1 (-2.36636) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98262 HOMO: -6.65863 LUMO: -0.46804 factor:1 | 1 (-1.40862) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.50858 HOMO: -7.24367 LUMO: 0.29388 factor:1 | 1 (-2.93458) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89207 HOMO: -7.02326 LUMO: -0.87893 factor:1 | 1 (-0.31807) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95945 HOMO: -6.88176 LUMO: 0.71566 factor:1 | 1 (-0.38545) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04459 HOMO: -6.46543 LUMO: 1.01498 factor:1 | 1 (-0.47059) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.46258 HOMO: -6.30760 LUMO: 0.17687 factor:1 | 1 (-1.88858) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.02156 HOMO: -6.73210 LUMO: -1.06941 factor:1 | 1 (-1.44756) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.35060 HOMO: -6.83550 LUMO: -0.75920 factor:1 | 1 (-1.77660) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.32037 HOMO: -6.94707 LUMO: 0.42178 factor:1 | 1 (-1.74637) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.64304 HOMO: -6.77019 LUMO: -0.38096 factor:1 | 1 (-3.06904) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.88966 HOMO: -7.34163 LUMO: 0.35103 factor:1 | 1 (-2.31566) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.98789 HOMO: -6.87632 LUMO: -0.87349 factor:1 | 1 (-2.41389) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07847 HOMO: -7.06952 LUMO: -1.47214 factor:1 | 1 (-0.50447) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10685 HOMO: -6.58788 LUMO: -0.37824 factor:1 | 1 (-0.53285) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76061 HOMO: -6.92802 LUMO: -1.24900 factor:1 | 1 (-0.18662) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92005 HOMO: -7.01237 LUMO: -1.31975 factor:1 | 1 (-0.34605) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73359 HOMO: -6.74842 LUMO: 0.45987 factor:1 | 1 (-0.15959) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.57944 HOMO: -6.53890 LUMO: 0.94424 factor:1 | -1 (2.99456) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.42093 HOMO: -6.52257 LUMO: -0.66940 factor:1 | -1 (0.15306) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01735 HOMO: -6.56883 LUMO: -1.48302 factor:1 | 1 (-0.44336) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.70760 HOMO: -7.21646 LUMO: 0.13061 factor:1 | -1 (1.86640) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.65239 HOMO: -6.62597 LUMO: -0.64763 factor:1 | -1 (1.92161) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.62727 HOMO: -7.38789 LUMO: 0.31021 factor:1 | -1 (1.94673) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80679 HOMO: -6.74570 LUMO: -0.70750 factor:1 | 1 (-0.23279) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09112 HOMO: -6.95251 LUMO: -1.25989 factor:1 | 1 (-0.51713) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44937 HOMO: -7.13483 LUMO: -0.76736 factor:1 | -1 (0.12463) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29837 HOMO: -6.93618 LUMO: -1.24628 factor:1 | -1 (0.27562) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76638 HOMO: -7.03686 LUMO: 0.26395 factor:1 | 1 (-0.19238) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86783 HOMO: -6.52257 LUMO: -0.84355 factor:1 | 1 (-0.29383) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31834 HOMO: -6.83278 LUMO: -0.49525 factor:1 | 1 (-0.74434) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67351 HOMO: -7.18381 LUMO: -1.64629 factor:1 | 1 (-0.09951) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.34134 HOMO: -6.74842 LUMO: -0.81090 factor:1 | -1 (0.23266) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73803 HOMO: -7.09401 LUMO: -0.92519 factor:1 | 1 (-0.16403) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.21527 HOMO: -7.20285 LUMO: -0.81634 factor:1 | -1 (0.35873) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.31783 HOMO: -6.72665 LUMO: 0.77008 factor:1 | -1 (0.25617) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00704 HOMO: -6.80829 LUMO: 0.86532 factor:1 | 1 (-0.43304) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11944.33751 HOMO: -6.20964 LUMO: 0.99866 factor:1 | -1 (4.23649) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07934 HOMO: -6.52801 LUMO: 1.07757 factor:1 | 1 (-0.50534) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56339 HOMO: -6.74298 LUMO: -0.67756 factor:1 | -1 (0.01061) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70731 HOMO: -7.43959 LUMO: 0.03265 factor:1 | 1 (-0.13331) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.01287 HOMO: -6.46815 LUMO: -0.29933 factor:1 | -1 (0.56113) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12451 HOMO: -6.70489 LUMO: -0.97145 factor:1 | 1 (-0.55051) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54094 HOMO: -6.30216 LUMO: -1.39322 factor:1 | -1 (0.03306) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80794 HOMO: -7.01782 LUMO: -1.07485 factor:1 | 1 (-0.23394) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.53965 HOMO: -6.93074 LUMO: 0.25851 factor:1 | -1 (2.03435) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.80749 HOMO: -7.07224 LUMO: 0.09524 factor:1 | -1 (1.76651) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05178 HOMO: -6.62325 LUMO: -0.45443 factor:1 | 1 (-0.47778) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99662 HOMO: -7.09945 LUMO: -1.20274 factor:1 | 1 (-0.42262) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98589 HOMO: -6.56067 LUMO: -1.39322 factor:1 | 1 (-1.41189) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01969 HOMO: -6.75387 LUMO: -0.72654 factor:1 | 1 (-1.44569) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.37037 HOMO: -6.28583 LUMO: -2.35651 factor:1 | 1 (-0.79637) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74246 HOMO: -6.55522 LUMO: -1.33608 factor:1 | 1 (-0.16847) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.17641 HOMO: -7.19741 LUMO: -0.93607 factor:1 | -1 (0.39759) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.57950 HOMO: -6.39740 LUMO: -1.14832 factor:1 | -1 (0.99449) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.04725 HOMO: -7.11850 LUMO: -0.97417 factor:1 | 1 (-1.47325) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50583 HOMO: -6.57699 LUMO: -1.14016 factor:1 | 1 (-0.93183) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64830 HOMO: -6.57699 LUMO: -1.31975 factor:1 | 1 (-1.07431) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72505 HOMO: -6.69128 LUMO: -0.76736 factor:1 | 1 (-0.15105) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15600 HOMO: -7.25728 LUMO: 0.29660 factor:1 | -1 (0.41799) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.49722 HOMO: -6.37019 LUMO: -0.95240 factor:1 | -1 (1.07678) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.76865 HOMO: -6.48447 LUMO: -0.55511 factor:1 | -1 (0.80535) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.70530 HOMO: -6.37291 LUMO: -0.78641 factor:1 | -1 (0.86870) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.96000 HOMO: -6.65863 LUMO: -0.69933 factor:1 | -1 (0.61400) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.03306 HOMO: -6.44638 LUMO: -0.16055 factor:1 | -1 (0.54094) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54867 HOMO: -6.41917 LUMO: -0.20136 factor:1 | -1 (0.02533) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88922 HOMO: -7.33347 LUMO: 0.12789 factor:1 | 1 (-0.31522) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03099 HOMO: -6.70489 LUMO: -0.52518 factor:1 | 1 (-0.45699) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15507 HOMO: -7.25183 LUMO: 0.32109 factor:1 | 1 (-0.58107) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69226 HOMO: -7.29265 LUMO: 0.28028 factor:1 | 1 (-0.11826) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05905 HOMO: -6.57155 LUMO: -0.51702 factor:1 | -1 (0.51495) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.04381 HOMO: -7.08040 LUMO: 0.39729 factor:1 | -1 (0.53019) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.48051 HOMO: -6.24501 LUMO: -0.44627 factor:1 | 1 (-1.90651) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.37033 HOMO: -6.73754 LUMO: -0.45443 factor:1 | 1 (-1.79633) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73505 HOMO: -6.24501 LUMO: 0.38096 factor:1 | 1 (-1.16106) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.15234 HOMO: -6.86815 LUMO: -0.91974 factor:1 | 1 (-1.57834) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.29749 HOMO: -7.40150 LUMO: 0.36191 factor:1 | 1 (-1.72349) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02696 HOMO: -6.44094 LUMO: -0.64219 factor:1 | 1 (-0.45296) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44839 HOMO: -6.69944 LUMO: -0.80001 factor:1 | -1 (0.12561) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09197 HOMO: -6.61509 LUMO: -0.70750 factor:1 | 1 (-0.51797) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98459 HOMO: -7.52123 LUMO: 0.06803 factor:1 | 1 (-0.41059) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16666 HOMO: -7.34163 LUMO: 0.30477 factor:1 | 1 (-0.59266) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.18020 HOMO: -6.68584 LUMO: -0.78641 factor:1 | -1 (0.39380) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05946 HOMO: -6.53890 LUMO: -0.50885 factor:1 | -1 (0.51454) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04432 HOMO: -6.75659 LUMO: -0.68845 factor:1 | 1 (-0.47032) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47076 HOMO: -7.08857 LUMO: 0.43266 factor:1 | -1 (0.10324) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65913 HOMO: -6.28583 LUMO: -0.46804 factor:1 | 1 (-1.08514) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90826 HOMO: -6.50080 LUMO: -0.24762 factor:1 | 1 (-0.33426) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62042 HOMO: -6.45454 LUMO: -0.58504 factor:1 | 1 (-0.04642) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57599 HOMO: -7.20558 LUMO: 0.20953 factor:1 | 1 (-0.00199) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13695 HOMO: -6.35930 LUMO: -0.20681 factor:1 | 1 (-0.56295) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57021 HOMO: -6.36202 LUMO: -0.14422 factor:1 | 1 (-0.99621) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75830 HOMO: -6.20692 LUMO: 1.97827 factor:1 | 1 (-0.18430) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47435 HOMO: -6.48719 LUMO: 1.74153 factor:1 | -1 (0.09965) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.09242 HOMO: -6.84638 LUMO: 1.88575 factor:1 | 1 (-1.51842) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.25733 HOMO: -5.90759 LUMO: 2.00820 factor:1 | 1 (-0.68333) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00896 HOMO: -6.56339 LUMO: 1.99732 factor:1 | 1 (-1.43497) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39690 HOMO: -6.20692 LUMO: 1.75241 factor:1 | 1 (-0.82290) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01504 HOMO: -6.16882 LUMO: 1.94017 factor:1 | 1 (-0.44104) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97579 HOMO: -6.80829 LUMO: 1.78507 factor:1 | 1 (-1.40179) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.70906 HOMO: -6.58243 LUMO: 1.78235 factor:1 | 1 (-2.13506) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91283 HOMO: -5.85045 LUMO: 1.82316 factor:1 | 1 (-1.33883) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85963 HOMO: -5.93752 LUMO: 1.56465 factor:1 | 1 (-1.28563) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.65477 HOMO: -6.59604 LUMO: -0.53334 factor:1 | 1 (-2.08077) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.61923 HOMO: -7.06135 LUMO: 0.29660 factor:1 | 1 (-2.04523) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.20880 HOMO: -6.50352 LUMO: 1.61908 factor:1 | -1 (1.36520) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.33654 HOMO: -6.68040 LUMO: -0.60681 factor:1 | -1 (2.23746) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.32862 HOMO: -6.93618 LUMO: -1.09662 factor:1 | -1 (2.24537) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.93193 HOMO: -6.72121 LUMO: -1.14016 factor:1 | -1 (1.64207) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.03568 HOMO: -7.12394 LUMO: -1.24900 factor:1 | -1 (1.53831) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.98119 HOMO: -6.71305 LUMO: -0.71566 factor:1 | -1 (2.59281) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01871 HOMO: -7.09401 LUMO: -0.86532 factor:1 | 1 (-0.44472) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.42850 HOMO: -7.08584 LUMO: -0.92519 factor:1 | -1 (0.14550) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93041 HOMO: -7.05591 LUMO: 0.11973 factor:1 | 1 (-0.35641) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38444 HOMO: -7.14843 LUMO: -1.58370 factor:1 | -1 (0.18955) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19006 HOMO: -7.36884 LUMO: -1.97010 factor:1 | 1 (-0.61607) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.95333 HOMO: -6.81373 LUMO: -1.72248 factor:1 | -1 (0.62066) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.51950 HOMO: -6.87360 LUMO: -1.03947 factor:1 | -1 (1.05450) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.06736 HOMO: -7.02870 LUMO: -0.87349 factor:1 | -1 (1.50664) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.13800 HOMO: -7.16476 LUMO: -1.18097 factor:1 | -1 (1.43600) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.02978 HOMO: -7.51851 LUMO: 0.07891 factor:1 | -1 (1.54422) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97939 HOMO: -7.04231 LUMO: -0.83539 factor:1 | 1 (-0.40540) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15794 HOMO: -6.83278 LUMO: -0.60137 factor:1 | -1 (0.41606) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.01687 HOMO: -6.89809 LUMO: -1.19186 factor:1 | -1 (0.55713) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.08535 HOMO: -7.16476 LUMO: -0.79185 factor:1 | -1 (1.48865) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.98219 HOMO: -6.97156 LUMO: -1.25444 factor:1 | -1 (1.59181) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59283 HOMO: -6.84366 LUMO: -0.88437 factor:1 | 1 (-0.01883) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85670 HOMO: -6.91986 LUMO: -1.12655 factor:1 | 1 (-0.28270) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.06447 HOMO: -6.49536 LUMO: -0.29660 factor:1 | -1 (0.50953) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.79350 HOMO: -6.74842 LUMO: 0.42450 factor:1 | -1 (1.78050) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84363 HOMO: -7.34435 LUMO: 0.32109 factor:1 | 1 (-1.26963) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14478 HOMO: -7.16476 LUMO: 0.28572 factor:1 | 1 (-0.57079) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96334 HOMO: -6.74298 LUMO: -0.43538 factor:1 | 1 (-0.38934) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12206 HOMO: -7.19469 LUMO: -1.61091 factor:1 | 1 (-0.54806) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82355 HOMO: -7.35252 LUMO: -1.78235 factor:1 | 1 (-1.24955) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81484 HOMO: -7.25456 LUMO: -1.66806 factor:1 | 1 (-1.24084) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45834 HOMO: -7.54844 LUMO: -1.07213 factor:1 | 1 (-0.88434) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64176 HOMO: -7.21918 LUMO: -1.55377 factor:1 | 1 (-0.06776) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.07701 HOMO: -7.01782 LUMO: -1.60547 factor:1 | -1 (0.49699) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75147 HOMO: -7.21646 LUMO: -1.53472 factor:1 | 1 (-0.17747) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.53888 HOMO: -6.73754 LUMO: -1.37417 factor:1 | -1 (1.03512) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.91844 HOMO: -6.78924 LUMO: 0.66396 factor:1 | -1 (2.65556) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.35428 HOMO: -6.82734 LUMO: 0.61226 factor:1 | -1 (2.21971) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.43194 HOMO: -6.74026 LUMO: 0.65579 factor:1 | -1 (1.14206) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.76776 HOMO: -7.10489 LUMO: -1.30887 factor:1 | -1 (1.80624) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.84092 HOMO: -7.05047 LUMO: 0.42722 factor:1 | -1 (0.73307) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.72577 HOMO: -6.61237 LUMO: 1.30887 factor:1 | -1 (0.84823) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51520 HOMO: -7.05863 LUMO: 0.59049 factor:1 | -1 (0.05880) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74023 HOMO: -6.26406 LUMO: 0.78641 factor:1 | 1 (-0.16623) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.59205 HOMO: -6.70489 LUMO: 0.67756 factor:1 | -1 (0.98195) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13160 HOMO: -6.78652 LUMO: -0.94968 factor:1 | -1 (0.44240) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54124 HOMO: -6.36202 LUMO: -0.94424 factor:1 | -1 (0.03276) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48673 HOMO: -6.81645 LUMO: -1.09934 factor:1 | -1 (0.08727) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70860 HOMO: -7.07224 LUMO: 0.85988 factor:1 | 1 (-1.13461) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12269 HOMO: -7.02326 LUMO: 1.10206 factor:1 | 1 (-0.54869) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78812 HOMO: -6.71305 LUMO: 0.84627 factor:1 | 1 (-1.21412) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14843 HOMO: -7.27360 LUMO: 0.88165 factor:1 | 1 (-0.57443) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43464 HOMO: -6.84911 LUMO: 0.59865 factor:1 | 1 (-0.86064) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66946 HOMO: -6.75114 LUMO: -2.49801 factor:1 | 1 (-0.09546) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73629 HOMO: -6.97156 LUMO: 0.53606 factor:1 | 1 (-0.16229) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53547 HOMO: -6.54434 LUMO: 0.73199 factor:1 | -1 (0.03853) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.87763 HOMO: -6.21236 LUMO: 0.99866 factor:1 | -1 (0.69637) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.56848 HOMO: -6.34025 LUMO: 0.50341 factor:1 | -1 (1.00552) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45574 HOMO: -6.59876 LUMO: -0.69389 factor:1 | -1 (0.11826) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.41662 HOMO: -6.54978 LUMO: -1.00682 factor:1 | -1 (1.15738) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.60887 HOMO: -6.82462 LUMO: -0.98777 factor:1 | -1 (0.96513) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.14848 HOMO: -6.85455 LUMO: -0.68573 factor:1 | -1 (2.42551) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.74850 HOMO: -7.55388 LUMO: -0.03265 factor:1 | -1 (1.82550) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.98674 HOMO: -6.77019 LUMO: -0.71838 factor:1 | -1 (2.58726) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.58585 HOMO: -6.84911 LUMO: -1.25444 factor:1 | -1 (1.98815) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.35709 HOMO: -6.95251 LUMO: -1.03675 factor:1 | -1 (2.21691) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.70874 HOMO: -6.80829 LUMO: -0.77280 factor:1 | -1 (1.86526) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.83345 HOMO: -6.94162 LUMO: -0.94151 factor:1 | -1 (1.74055) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.33880 HOMO: -6.89809 LUMO: -0.90886 factor:1 | -1 (2.23520) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.70343 HOMO: -6.85183 LUMO: -0.88981 factor:1 | -1 (1.87057) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.70266 HOMO: -6.51985 LUMO: -0.84627 factor:1 | -1 (0.87134) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.25131 HOMO: -6.83278 LUMO: -1.08029 factor:1 | -1 (1.32269) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.99778 HOMO: -6.91986 LUMO: 0.66396 factor:1 | -1 (1.57622) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.49423 HOMO: -6.94162 LUMO: 0.50885 factor:1 | -1 (2.07977) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.11077 HOMO: -6.94435 LUMO: 0.80546 factor:1 | -1 (2.46323) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.45197 HOMO: -6.74298 LUMO: -0.81634 factor:1 | -1 (2.12203) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.99484 HOMO: -7.04503 LUMO: 1.15921 factor:1 | -1 (1.57916) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.58406 HOMO: -6.76475 LUMO: 0.75920 factor:1 | -1 (1.98994) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.32854 HOMO: -7.05047 LUMO: 0.68845 factor:1 | -1 (2.24546) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.98214 HOMO: -7.12666 LUMO: 0.60681 factor:1 | -1 (2.59186) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.52622 HOMO: -6.90897 LUMO: -1.22723 factor:1 | -1 (1.04777) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.62332 HOMO: -7.10761 LUMO: 0.58232 factor:1 | -1 (1.95068) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.10145 HOMO: -6.57427 LUMO: 0.71294 factor:1 | -1 (1.47254) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.52617 HOMO: -6.22597 LUMO: 0.99322 factor:1 | -1 (1.04783) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.02529 HOMO: -6.83550 LUMO: -0.77825 factor:1 | -1 (1.54871) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.50557 HOMO: -7.14843 LUMO: 0.44627 factor:1 | -1 (1.06843) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.86185 HOMO: -7.08040 LUMO: 0.78913 factor:1 | -1 (0.71215) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.96314 HOMO: -6.81373 LUMO: -0.93879 factor:1 | -1 (1.61086) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.60087 HOMO: -6.95251 LUMO: 0.22585 factor:1 | -1 (0.97313) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81243 HOMO: -7.13483 LUMO: -1.25444 factor:1 | -1 (0.76157) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.16600 HOMO: -6.37835 LUMO: -1.54289 factor:1 | -1 (1.40800) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.00668 HOMO: -6.53617 LUMO: -1.43948 factor:1 | -1 (1.56732) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52292 HOMO: -6.38379 LUMO: 0.16055 factor:1 | -1 (0.05108) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51672 HOMO: -6.53617 LUMO: 0.15783 factor:1 | -1 (0.05728) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.41089 HOMO: -6.79740 LUMO: -0.17960 factor:1 | -1 (0.16311) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.17745 HOMO: -6.26678 LUMO: -0.41361 factor:1 | -1 (0.39655) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.47472 HOMO: -6.35658 LUMO: -0.24218 factor:1 | -1 (2.09928) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.38011 HOMO: -6.48175 LUMO: -0.71566 factor:1 | -1 (2.19389) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.91070 HOMO: -6.21508 LUMO: -0.40001 factor:1 | -1 (1.66330) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.09797 HOMO: -6.51985 LUMO: -0.32654 factor:1 | -1 (1.47603) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.99685 HOMO: -6.45182 LUMO: -0.66396 factor:1 | -1 (1.57714) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.98172 HOMO: -6.51441 LUMO: -0.65307 factor:1 | -1 (1.59227) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05195 HOMO: -6.57971 LUMO: -0.92519 factor:1 | -1 (0.52205) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.21306 HOMO: -6.67223 LUMO: -0.58232 factor:1 | -1 (2.36094) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.47157 HOMO: -6.10351 LUMO: -0.45987 factor:1 | -1 (2.10243) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.17531 HOMO: -6.13889 LUMO: -0.50341 factor:1 | -1 (1.39869) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.28268 HOMO: -6.63141 LUMO: -0.28300 factor:1 | -1 (1.29132) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.74394 HOMO: -6.37563 LUMO: -0.22858 factor:1 | -1 (0.83006) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.85584 HOMO: -6.37019 LUMO: 0.11429 factor:1 | -1 (1.71815) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.88352 HOMO: -6.23957 LUMO: 0.28844 factor:1 | -1 (1.69048) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.21335 HOMO: -6.41372 LUMO: -0.53879 factor:1 | -1 (1.36065) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.35784 HOMO: -7.06680 LUMO: 0.32654 factor:1 | -1 (1.21616) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.80577 HOMO: -6.50896 LUMO: -0.73743 factor:1 | -1 (0.76823) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.28374 HOMO: -6.42189 LUMO: -0.28572 factor:1 | -1 (1.29026) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.77883 HOMO: -6.79740 LUMO: -0.25851 factor:1 | -1 (0.79517) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.15963 HOMO: -6.32393 LUMO: 0.17960 factor:1 | -1 (1.41437) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.60920 HOMO: -6.65046 LUMO: 0.03537 factor:1 | -1 (1.96480) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.24551 HOMO: -6.60148 LUMO: 0.07619 factor:1 | -1 (1.32849) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.43445 HOMO: -6.57971 LUMO: 0.11429 factor:1 | -1 (2.13955) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.60915 HOMO: -6.88448 LUMO: -1.21907 factor:1 | -1 (1.96485) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.70994 HOMO: -6.97700 LUMO: 0.36463 factor:1 | -1 (1.86406) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22079 HOMO: -6.73210 LUMO: -0.84083 factor:1 | 1 (-0.64679) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78317 HOMO: -6.21236 LUMO: -0.68845 factor:1 | 1 (-0.20917) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73468 HOMO: -6.35658 LUMO: -0.82995 factor:1 | 1 (-0.16068) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76883 HOMO: -6.75114 LUMO: -0.94424 factor:1 | 1 (-0.19483) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77368 HOMO: -6.74026 LUMO: -1.46125 factor:1 | 1 (-0.19968) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70529 HOMO: -7.06952 LUMO: 0.91974 factor:1 | 1 (-1.13129) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96652 HOMO: -7.08857 LUMO: 0.74559 factor:1 | 1 (-0.39252) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74262 HOMO: -6.74298 LUMO: 1.03131 factor:1 | 1 (-1.16862) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99885 HOMO: -6.74842 LUMO: -1.77962 factor:1 | 1 (-0.42485) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44697 HOMO: -6.82462 LUMO: -1.61908 factor:1 | 1 (-0.87297) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94885 HOMO: -7.17020 LUMO: -1.02043 factor:1 | 1 (-1.37486) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64357 HOMO: -6.26406 LUMO: -0.96328 factor:1 | 1 (-1.06957) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73193 HOMO: -6.50896 LUMO: -0.38640 factor:1 | 1 (-0.15793) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16283 HOMO: -7.27632 LUMO: -1.17553 factor:1 | 1 (-0.58883) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66127 HOMO: -6.54162 LUMO: -1.36873 factor:1 | 1 (-0.08727) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.11946 HOMO: -6.42733 LUMO: -1.15648 factor:1 | -1 (0.45454) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06734 HOMO: -6.73754 LUMO: -2.58780 factor:1 | 1 (-0.49334) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81723 HOMO: -7.20285 LUMO: 0.75103 factor:1 | 1 (-1.24323) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86678 HOMO: -6.98788 LUMO: 0.34831 factor:1 | 1 (-1.29279) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.18454 HOMO: -6.80013 LUMO: -1.11567 factor:1 | 1 (-0.61054) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81027 HOMO: -6.67767 LUMO: -0.82450 factor:1 | 1 (-1.23627) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23022 HOMO: -6.84911 LUMO: -0.21497 factor:1 | 1 (-1.65622) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03110 HOMO: -6.23141 LUMO: 0.21769 factor:1 | 1 (-0.45710) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30272 HOMO: -6.68312 LUMO: 0.16327 factor:1 | 1 (-0.72872) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17392 HOMO: -7.04503 LUMO: -1.04220 factor:1 | 1 (-1.59992) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57179 HOMO: -6.67495 LUMO: -0.71294 factor:1 | -1 (0.00220) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35241 HOMO: -6.70216 LUMO: -0.55239 factor:1 | 1 (-0.77841) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.65961 HOMO: -6.60420 LUMO: -0.71294 factor:1 | -1 (0.91438) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.54214 HOMO: -7.40694 LUMO: 0.11973 factor:1 | -1 (1.03186) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16666 HOMO: -6.58788 LUMO: -0.29116 factor:1 | 1 (-0.59266) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.25401 HOMO: -6.63686 LUMO: -0.32654 factor:1 | 1 (-0.68001) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77944 HOMO: -6.85183 LUMO: -0.95512 factor:1 | 1 (-0.20545) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96339 HOMO: -6.82189 LUMO: -0.88165 factor:1 | 1 (-0.38939) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69857 HOMO: -6.97428 LUMO: -1.03947 factor:1 | 1 (-0.12457) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68460 HOMO: -6.51441 LUMO: -0.05714 factor:1 | 1 (-1.11061) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.96865 HOMO: -6.61509 LUMO: -0.77008 factor:1 | -1 (0.60534) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.87880 HOMO: -7.36340 LUMO: 0.29116 factor:1 | -1 (0.69520) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.75869 HOMO: -6.64230 LUMO: -0.79185 factor:1 | -1 (0.81531) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.42687 HOMO: -6.56883 LUMO: -1.03403 factor:1 | -1 (0.14713) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.10773 HOMO: -6.69400 LUMO: -0.77825 factor:1 | -1 (0.46627) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69816 HOMO: -6.37019 LUMO: -0.79185 factor:1 | 1 (-0.12417) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91858 HOMO: -6.49808 LUMO: -0.94424 factor:1 | 1 (-0.34458) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84176 HOMO: -6.91713 LUMO: -0.75376 factor:1 | 1 (-0.26776) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10704 HOMO: -7.13755 LUMO: 0.41361 factor:1 | 1 (-0.53304) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.64297 HOMO: -7.12122 LUMO: 0.39457 factor:1 | -1 (1.93103) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59288 HOMO: -6.59332 LUMO: -0.57144 factor:1 | 1 (-0.01888) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.24200 HOMO: -6.62325 LUMO: -0.66940 factor:1 | -1 (1.33200) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.02052 HOMO: -6.90897 LUMO: -0.08708 factor:1 | -1 (0.55348) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05980 HOMO: -6.65591 LUMO: -0.81090 factor:1 | 1 (-0.48580) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81571 HOMO: -6.65318 LUMO: -0.94696 factor:1 | 1 (-1.24171) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.71220 HOMO: -6.96067 LUMO: -1.03675 factor:1 | 1 (-1.13820) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01711 HOMO: -6.23141 LUMO: -0.66396 factor:1 | 1 (-0.44311) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56311 HOMO: -6.52529 LUMO: -0.78369 factor:1 | -1 (0.01088) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.59502 HOMO: -6.39468 LUMO: -0.40817 factor:1 | -1 (1.97898) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57892 HOMO: -6.76203 LUMO: -0.20409 factor:1 | 1 (-0.00493) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.77518 HOMO: -6.96611 LUMO: -0.90342 factor:1 | -1 (0.79882) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.67444 HOMO: -6.54706 LUMO: -0.87893 factor:1 | -1 (0.89955) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33611 HOMO: -7.24367 LUMO: -0.97689 factor:1 | 1 (-0.76211) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.18673 HOMO: -6.61781 LUMO: 1.43404 factor:1 | -1 (0.38727) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80198 HOMO: -6.17971 LUMO: 1.79867 factor:1 | 1 (-0.22798) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.92550 HOMO: -5.73344 LUMO: 2.13609 factor:1 | -1 (0.64850) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.51433 HOMO: -6.72121 LUMO: 2.06807 factor:1 | -1 (1.05967) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38362 HOMO: -6.91169 LUMO: 2.02997 factor:1 | 1 (-0.80962) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95719 HOMO: -7.06408 LUMO: 1.41499 factor:1 | 1 (-0.38319) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79670 HOMO: -6.94162 LUMO: -0.90070 factor:1 | 1 (-0.22270) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41328 HOMO: -7.09401 LUMO: 0.35103 factor:1 | 1 (-0.83928) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89825 HOMO: -6.78652 LUMO: 0.91974 factor:1 | 1 (-0.32425) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39042 HOMO: -6.32937 LUMO: -1.89119 factor:1 | 1 (-0.81642) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56181 HOMO: -7.12666 LUMO: -1.06397 factor:1 | -1 (0.01219) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.97402 HOMO: -6.38107 LUMO: -1.43132 factor:1 | -1 (1.59998) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.08137 HOMO: -7.09129 LUMO: 0.08980 factor:1 | -1 (1.49263) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.98700 HOMO: -6.31304 LUMO: -0.57960 factor:1 | -1 (1.58700) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.16668 HOMO: -6.94435 LUMO: -0.74287 factor:1 | -1 (1.40732) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.38794 HOMO: -6.35658 LUMO: -1.53472 factor:1 | -1 (2.18605) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.20127 HOMO: -6.39740 LUMO: -1.48846 factor:1 | -1 (2.37272) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.44680 HOMO: -7.05319 LUMO: -0.33198 factor:1 | -1 (2.12720) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.74005 HOMO: -6.68040 LUMO: -0.09252 factor:1 | -1 (0.83395) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.35520 HOMO: -6.35930 LUMO: -0.43266 factor:1 | -1 (1.21880) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.95576 HOMO: -6.59604 LUMO: -1.45853 factor:1 | -1 (1.61823) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94451 HOMO: -6.46270 LUMO: -1.49391 factor:1 | 1 (-0.37051) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85341 HOMO: -7.05863 LUMO: -1.04764 factor:1 | 1 (-0.27941) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88247 HOMO: -7.14027 LUMO: -0.81634 factor:1 | 1 (-0.30847) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33347 HOMO: -6.80285 LUMO: -0.74287 factor:1 | 1 (-0.75947) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99939 HOMO: -6.53890 LUMO: -1.13471 factor:1 | 1 (-0.42540) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.62481 HOMO: -6.49808 LUMO: -1.35513 factor:1 | -1 (0.94919) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.28353 HOMO: -6.75931 LUMO: -1.49663 factor:1 | -1 (1.29047) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.18428 HOMO: -6.84638 LUMO: -0.77552 factor:1 | -1 (0.38972) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.61048 HOMO: -6.65863 LUMO: -1.34696 factor:1 | -1 (1.96352) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.17512 HOMO: -6.25590 LUMO: -2.36467 factor:1 | -1 (1.39888) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59133 HOMO: -7.24911 LUMO: 0.33470 factor:1 | 1 (-0.01733) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48480 HOMO: -6.65863 LUMO: -0.75648 factor:1 | -1 (0.08920) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.20147 HOMO: -6.31576 LUMO: -0.83267 factor:1 | -1 (2.37253) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.10149 HOMO: -6.64774 LUMO: -0.66124 factor:1 | -1 (2.47251) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.23022 HOMO: -6.75387 LUMO: -1.00138 factor:1 | -1 (1.34378) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.76888 HOMO: -6.52529 LUMO: -0.68301 factor:1 | -1 (1.80512) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38453 HOMO: -6.59332 LUMO: -0.68028 factor:1 | -1 (0.18947) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.52448 HOMO: -5.98650 LUMO: 0.31565 factor:1 | -1 (1.04952) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.25750 HOMO: -6.59876 LUMO: 0.22585 factor:1 | -1 (0.31650) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.47934 HOMO: -6.72121 LUMO: 0.10340 factor:1 | -1 (1.09466) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.23521 HOMO: -6.09807 LUMO: 0.20136 factor:1 | -1 (2.33879) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.23344 HOMO: -6.31576 LUMO: 0.06259 factor:1 | -1 (2.34056) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.09880 HOMO: -6.35658 LUMO: -0.58232 factor:1 | -1 (2.47520) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64276 HOMO: -6.34842 LUMO: -0.55783 factor:1 | 1 (-0.06876) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07012 HOMO: -6.47359 LUMO: -0.57144 factor:1 | 1 (-0.49612) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15674 HOMO: -6.42189 LUMO: -0.09796 factor:1 | -1 (0.41726) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.56169 HOMO: -6.35658 LUMO: -0.31293 factor:1 | 1 (-0.98769) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82832 HOMO: -7.35524 LUMO: 0.10340 factor:1 | 1 (-0.25432) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.27017 HOMO: -7.10217 LUMO: 0.36463 factor:1 | 1 (-0.69618) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04035 HOMO: -6.43549 LUMO: -0.56872 factor:1 | 1 (-0.46635) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95224 HOMO: -6.50080 LUMO: -0.71294 factor:1 | 1 (-0.37824) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75291 HOMO: -6.59060 LUMO: -0.57960 factor:1 | 1 (-0.17891) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72520 HOMO: -6.78924 LUMO: -0.31565 factor:1 | 1 (-1.15120) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92015 HOMO: -6.35658 LUMO: 0.07891 factor:1 | 1 (-0.34616) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05437 HOMO: -6.74026 LUMO: -0.87621 factor:1 | -1 (0.51963) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97882 HOMO: -6.54434 LUMO: 0.81906 factor:1 | 1 (-0.40482) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.00774 HOMO: -6.66135 LUMO: 1.40955 factor:1 | -1 (1.56626) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.02243 HOMO: -6.73754 LUMO: -2.54971 factor:1 | -1 (1.55157) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.39901 HOMO: -6.65318 LUMO: 0.69389 factor:1 | -1 (1.17499) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.87630 HOMO: -6.73482 LUMO: 0.62858 factor:1 | -1 (0.69770) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.32595 HOMO: -6.83550 LUMO: 0.68573 factor:1 | -1 (1.24805) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.71652 HOMO: -6.83278 LUMO: 0.45987 factor:1 | -1 (1.85748) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.97517 HOMO: -6.78380 LUMO: 0.68301 factor:1 | -1 (1.59883) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.06058 HOMO: -6.90625 LUMO: 1.36601 factor:1 | -1 (1.51342) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.73475 HOMO: -6.82734 LUMO: 1.48302 factor:1 | -1 (1.83924) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.39663 HOMO: -6.44094 LUMO: -0.94424 factor:1 | -1 (2.17737) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.10759 HOMO: -6.91441 LUMO: 0.28844 factor:1 | -1 (2.46641) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.35164 HOMO: -6.49808 LUMO: -0.51157 factor:1 | -1 (1.22236) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.86656 HOMO: -7.09673 LUMO: -0.06259 factor:1 | -1 (0.70744) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.84627 HOMO: -6.77019 LUMO: 0.92247 factor:1 | -1 (1.72773) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.70104 HOMO: -6.75931 LUMO: 1.13744 factor:1 | -1 (1.87296) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.99646 HOMO: -6.15794 LUMO: 1.12383 factor:1 | -1 (0.57753) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.63685 HOMO: -6.59604 LUMO: 1.19458 factor:1 | -1 (1.93715) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.37234 HOMO: -7.09401 LUMO: 0.60137 factor:1 | -1 (0.20166) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.16745 HOMO: -6.34025 LUMO: 0.48164 factor:1 | -1 (2.40655) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.87836 HOMO: -6.72665 LUMO: -2.47624 factor:1 | -1 (2.69564) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.75553 HOMO: -6.48175 LUMO: 0.58232 factor:1 | -1 (2.81847) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.71600 HOMO: -6.94162 LUMO: 0.28300 factor:1 | -1 (0.85800) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.94464 HOMO: -6.65591 LUMO: 0.57144 factor:1 | -1 (1.62936) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.18211 HOMO: -6.58788 LUMO: -1.03947 factor:1 | -1 (1.39189) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.09508 HOMO: -7.18108 LUMO: 0.37824 factor:1 | -1 (0.47892) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.31803 HOMO: -6.63958 LUMO: -1.52112 factor:1 | -1 (1.25597) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.74118 HOMO: -6.12528 LUMO: -0.53606 factor:1 | -1 (1.83282) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06538 HOMO: -6.22324 LUMO: -0.87893 factor:1 | 1 (-0.49138) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59833 HOMO: -6.62053 LUMO: -0.91974 factor:1 | 1 (-0.02433) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01937 HOMO: -6.84366 LUMO: -0.83811 factor:1 | 1 (-0.44537) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92129 HOMO: -7.26000 LUMO: 0.25851 factor:1 | 1 (-1.34729) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09284 HOMO: -6.49536 LUMO: -0.63403 factor:1 | 1 (-0.51884) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66523 HOMO: -6.45726 LUMO: -0.77825 factor:1 | 1 (-1.09123) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92669 HOMO: -6.74570 LUMO: -0.75103 factor:1 | 1 (-0.35269) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65710 HOMO: -7.20285 LUMO: 0.10612 factor:1 | 1 (-0.08310) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.09607 HOMO: -6.45182 LUMO: -0.56600 factor:1 | -1 (1.47793) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.10028 HOMO: -6.83278 LUMO: -0.71838 factor:1 | -1 (1.47371) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.05724 HOMO: -7.01510 LUMO: -1.09662 factor:1 | -1 (1.51676) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.01347 HOMO: -6.48719 LUMO: 0.16871 factor:1 | -1 (0.56053) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.49169 HOMO: -7.30898 LUMO: 0.26667 factor:1 | -1 (1.08231) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20231 HOMO: -6.68856 LUMO: -0.78641 factor:1 | 1 (-0.62831) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76929 HOMO: -6.56883 LUMO: -1.00682 factor:1 | 1 (-1.19529) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21777 HOMO: -6.41100 LUMO: -0.48980 factor:1 | 1 (-0.64377) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89846 HOMO: -6.52257 LUMO: -0.59865 factor:1 | 1 (-1.32446) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.12235 HOMO: -6.63686 LUMO: -0.56055 factor:1 | 1 (-1.54836) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.71451 HOMO: -6.79740 LUMO: -0.75376 factor:1 | 1 (-1.14051) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.03306 HOMO: -5.89127 LUMO: 0.22313 factor:1 | -1 (0.54094) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.17864 HOMO: -6.34842 LUMO: 0.11429 factor:1 | -1 (0.39535) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.18450 HOMO: -6.13617 LUMO: 1.94834 factor:1 | -1 (0.38950) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83939 HOMO: -6.50080 LUMO: 1.74153 factor:1 | 1 (-0.26539) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15619 HOMO: -6.33481 LUMO: 1.68438 factor:1 | 1 (-0.58219) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99975 HOMO: -6.53073 LUMO: 1.95106 factor:1 | 1 (-0.42575) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14454 HOMO: -6.46270 LUMO: 1.89935 factor:1 | 1 (-0.57054) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95738 HOMO: -5.87222 LUMO: 1.91568 factor:1 | 1 (-0.38338) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63813 HOMO: -6.07630 LUMO: 1.81500 factor:1 | 1 (-1.06413) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05278 HOMO: -6.20964 LUMO: 1.81500 factor:1 | 1 (-0.47878) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86473 HOMO: -6.15522 LUMO: 1.90752 factor:1 | 1 (-0.29073) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70074 HOMO: -6.11984 LUMO: 1.95378 factor:1 | 1 (-1.12674) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.84816 HOMO: -6.58516 LUMO: 2.04358 factor:1 | -1 (0.72584) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.98207 HOMO: -7.37156 LUMO: 0.24490 factor:1 | -1 (0.59193) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.95257 HOMO: -6.36474 LUMO: -0.90070 factor:1 | -1 (0.62143) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.01162 HOMO: -6.43549 LUMO: -0.40817 factor:1 | -1 (0.56238) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.80145 HOMO: -7.32258 LUMO: 0.29388 factor:1 | -1 (1.77255) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.05871 HOMO: -6.41372 LUMO: -0.20409 factor:1 | -1 (1.51529) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.84899 HOMO: -7.18381 LUMO: 0.42722 factor:1 | -1 (1.72501) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.11407 HOMO: -6.53890 LUMO: -0.54151 factor:1 | -1 (0.45993) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15924 HOMO: -6.61509 LUMO: 0.08708 factor:1 | -1 (0.41476) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81762 HOMO: -6.78108 LUMO: 2.03541 factor:1 | 1 (-0.24362) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.55213 HOMO: -6.50896 LUMO: 1.53472 factor:1 | -1 (1.02187) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06465 HOMO: -6.65591 LUMO: 1.80411 factor:1 | 1 (-0.49065) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08715 HOMO: -6.64502 LUMO: 1.52112 factor:1 | 1 (-0.51315) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.64868 HOMO: -6.72938 LUMO: 1.48030 factor:1 | -1 (1.92531) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.84235 HOMO: -6.16882 LUMO: 1.96466 factor:1 | -1 (1.73165) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.81650 HOMO: -6.22597 LUMO: 1.43132 factor:1 | -1 (1.75750) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.58819 HOMO: -6.57699 LUMO: 2.05718 factor:1 | -1 (1.98581) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.32866 HOMO: -6.52529 LUMO: 1.89663 factor:1 | -1 (0.24534) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29361 HOMO: -6.30760 LUMO: 1.88031 factor:1 | -1 (0.28039) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71830 HOMO: -6.14977 LUMO: 1.92657 factor:1 | 1 (-0.14430) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.74775 HOMO: -6.20964 LUMO: 1.83949 factor:1 | -1 (0.82625) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84614 HOMO: -6.31848 LUMO: 1.91296 factor:1 | 1 (-0.27214) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.97423 HOMO: -5.80691 LUMO: 2.19868 factor:1 | -1 (0.59977) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.69635 HOMO: -6.00827 LUMO: 2.15514 factor:1 | -1 (0.87765) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.86215 HOMO: -6.51713 LUMO: 2.08711 factor:1 | -1 (0.71185) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.74155 HOMO: -6.32937 LUMO: 2.11705 factor:1 | -1 (0.83245) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.80079 HOMO: -6.26678 LUMO: 1.95922 factor:1 | -1 (0.77321) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.71352 HOMO: -6.43005 LUMO: 2.56603 factor:1 | -1 (0.86048) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.75390 HOMO: -6.41644 LUMO: 2.68304 factor:1 | -1 (0.82010) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81298 HOMO: -5.97834 LUMO: 2.02997 factor:1 | -1 (0.76102) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.39844 HOMO: -6.14161 LUMO: 1.77690 factor:1 | -1 (1.17556) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.75504 HOMO: -6.21508 LUMO: 1.80411 factor:1 | -1 (0.81895) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.68759 HOMO: -6.46270 LUMO: 2.34562 factor:1 | -1 (0.88641) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.52541 HOMO: -6.39195 LUMO: -0.75920 factor:1 | -1 (1.04859) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.76498 HOMO: -7.08584 LUMO: -1.14016 factor:1 | -1 (0.80902) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.67493 HOMO: -6.70216 LUMO: -0.65035 factor:1 | -1 (0.89906) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.54516 HOMO: -6.79468 LUMO: -0.83811 factor:1 | -1 (1.02884) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.85472 HOMO: -6.99877 LUMO: -0.79729 factor:1 | -1 (0.71928) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.86751 HOMO: -7.08040 LUMO: -0.85444 factor:1 | -1 (0.70649) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47127 HOMO: -7.39333 LUMO: 0.12789 factor:1 | 1 (-0.89727) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35851 HOMO: -7.05047 LUMO: 0.13878 factor:1 | -1 (0.21549) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72856 HOMO: -6.90897 LUMO: -0.77552 factor:1 | 1 (-0.15456) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.91842 HOMO: -7.25456 LUMO: 0.05170 factor:1 | -1 (0.65558) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.47251 HOMO: -6.84638 LUMO: -0.84355 factor:1 | -1 (1.10149) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.32566 HOMO: -6.78108 LUMO: -0.81634 factor:1 | 1 (-0.75166) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83315 HOMO: -6.74570 LUMO: -0.77280 factor:1 | 1 (-1.25915) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82102 HOMO: -7.28177 LUMO: -1.68438 factor:1 | 1 (-0.24702) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30307 HOMO: -7.22190 LUMO: -1.63540 factor:1 | 1 (-0.72907) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80918 HOMO: -7.15932 LUMO: -1.57554 factor:1 | 1 (-1.23518) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19442 HOMO: -6.57971 LUMO: -0.93063 factor:1 | 1 (-0.62042) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.56327 HOMO: -6.88176 LUMO: 0.58232 factor:1 | 1 (-0.98927) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05017 HOMO: -6.85727 LUMO: 0.51430 factor:1 | 1 (-0.47617) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84056 HOMO: -6.83550 LUMO: 0.87893 factor:1 | 1 (-0.26656) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76470 HOMO: -7.06680 LUMO: 0.87621 factor:1 | 1 (-0.19070) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12035 HOMO: -6.52257 LUMO: 0.81362 factor:1 | 1 (-0.54635) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.55527 HOMO: -6.95523 LUMO: 1.17009 factor:1 | -1 (2.01873) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.33428 HOMO: -7.21374 LUMO: 0.97145 factor:1 | -1 (1.23972) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.40051 HOMO: -6.81373 LUMO: -1.54561 factor:1 | -1 (1.17349) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.30848 HOMO: -6.86543 LUMO: -1.52656 factor:1 | -1 (1.26552) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.02828 HOMO: -6.90081 LUMO: -0.78097 factor:1 | -1 (1.54572) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.79315 HOMO: -6.64502 LUMO: -0.82723 factor:1 | -1 (1.78085) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.01503 HOMO: -6.65591 LUMO: -0.82178 factor:1 | -1 (1.55897) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.93536 HOMO: -6.79468 LUMO: -1.46397 factor:1 | -1 (1.63864) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.57119 HOMO: -7.25728 LUMO: 0.73743 factor:1 | -1 (2.00281) | 1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.46848 HOMO: -7.00149 LUMO: 1.30070 factor:1 | -1 (1.10552) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.43901 HOMO: -7.07768 LUMO: 0.78097 factor:1 | -1 (1.13499) | 1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.28562 HOMO: -6.86271 LUMO: 0.86260 factor:1 | -1 (1.28838) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.68352 HOMO: -6.94707 LUMO: 0.39729 factor:1 | -1 (1.89048) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.01794 HOMO: -6.79740 LUMO: 0.67484 factor:1 | -1 (1.55606) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.08374 HOMO: -6.91986 LUMO: -1.14288 factor:1 | -1 (1.49026) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.75994 HOMO: -6.31576 LUMO: 1.01771 factor:1 | -1 (0.81406) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.36377 HOMO: -6.81645 LUMO: 0.81362 factor:1 | -1 (1.21023) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.32347 HOMO: -6.92258 LUMO: -0.99594 factor:1 | -1 (1.25053) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92424 HOMO: -6.81373 LUMO: 0.61770 factor:1 | 1 (-0.35024) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60532 HOMO: -7.18653 LUMO: 1.19186 factor:1 | 1 (-0.03132) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64260 HOMO: -7.00693 LUMO: 0.45715 factor:1 | 1 (-0.06860) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71629 HOMO: -7.11306 LUMO: 0.53334 factor:1 | 1 (-0.14229) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82573 HOMO: -6.63414 LUMO: -1.64357 factor:1 | 1 (-0.25173) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73427 HOMO: -6.22052 LUMO: -0.74015 factor:1 | 1 (-0.16028) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85321 HOMO: -6.81101 LUMO: -0.50069 factor:1 | 1 (-1.27921) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16353 HOMO: -6.71849 LUMO: -0.51974 factor:1 | 1 (-0.58953) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00767 HOMO: -6.72121 LUMO: -1.77690 factor:1 | 1 (-0.43367) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89092 HOMO: -6.94162 LUMO: -1.78779 factor:1 | 1 (-1.31692) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20386 HOMO: -6.91169 LUMO: 0.88981 factor:1 | 1 (-0.62986) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83775 HOMO: -6.97428 LUMO: 0.70750 factor:1 | 1 (-1.26375) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91101 HOMO: -6.74842 LUMO: 1.15921 factor:1 | 1 (-0.33701) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48841 HOMO: -7.25183 LUMO: -0.99594 factor:1 | 1 (-0.91441) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92357 HOMO: -6.43821 LUMO: -1.00410 factor:1 | 1 (-1.34958) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95074 HOMO: -6.52257 LUMO: -0.68573 factor:1 | 1 (-0.37674) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15801 HOMO: -6.60148 LUMO: -0.52518 factor:1 | 1 (-0.58401) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92681 HOMO: -6.07086 LUMO: -1.39594 factor:1 | 1 (-1.35281) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47992 HOMO: -6.78108 LUMO: -1.54833 factor:1 | 1 (-0.90592) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28852 HOMO: -6.73482 LUMO: -1.01498 factor:1 | 1 (-0.71452) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64932 HOMO: -6.85183 LUMO: 1.06669 factor:1 | 1 (-0.07532) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13643 HOMO: -6.98516 LUMO: 1.43948 factor:1 | 1 (-0.56243) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92263 HOMO: -6.94162 LUMO: 0.79185 factor:1 | 1 (-0.34863) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88864 HOMO: -6.67495 LUMO: -1.06669 factor:1 | 1 (-0.31465) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.71688 HOMO: -6.88720 LUMO: -1.00682 factor:1 | 1 (-1.14288) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62784 HOMO: -6.85999 LUMO: -0.78097 factor:1 | 1 (-1.05384) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82331 HOMO: -6.51713 LUMO: -0.89798 factor:1 | 1 (-0.24931) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92941 HOMO: -6.63141 LUMO: -0.91430 factor:1 | 1 (-0.35541) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87968 HOMO: -6.63414 LUMO: 0.04354 factor:1 | 1 (-1.30568) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51725 HOMO: -6.65046 LUMO: -0.73743 factor:1 | 1 (-0.94326) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.17029 HOMO: -6.73754 LUMO: -0.71838 factor:1 | -1 (0.40371) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33439 HOMO: -6.65863 LUMO: -0.60137 factor:1 | 1 (-0.76039) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03700 HOMO: -6.61509 LUMO: -0.47892 factor:1 | 1 (-0.46300) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98846 HOMO: -6.82189 LUMO: -0.64763 factor:1 | 1 (-0.41446) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.30802 HOMO: -6.56883 LUMO: -0.51974 factor:1 | -1 (1.26598) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83697 HOMO: -6.97428 LUMO: -0.95512 factor:1 | 1 (-0.26297) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11814 HOMO: -6.70489 LUMO: -0.04082 factor:1 | 1 (-0.54415) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.00080 HOMO: -6.74026 LUMO: 0.02177 factor:1 | -1 (1.57320) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.72183 HOMO: -6.50080 LUMO: -0.89525 factor:1 | -1 (1.85217) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.58038 HOMO: -6.46815 LUMO: -0.61226 factor:1 | -1 (1.99361) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.38084 HOMO: -6.57971 LUMO: -0.64219 factor:1 | -1 (2.19316) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.40929 HOMO: -7.17836 LUMO: 0.37280 factor:1 | -1 (0.16471) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.50590 HOMO: -6.67223 LUMO: 0.12245 factor:1 | -1 (1.06810) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76298 HOMO: -6.55250 LUMO: 0.22858 factor:1 | 1 (-0.18898) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.84555 HOMO: -6.97156 LUMO: -1.12927 factor:1 | -1 (0.72845) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06777 HOMO: -6.78924 LUMO: -0.84900 factor:1 | 1 (-1.49377) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39010 HOMO: -6.65046 LUMO: -0.65307 factor:1 | 1 (-0.81610) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.95729 HOMO: -7.41782 LUMO: 0.08980 factor:1 | 1 (-1.38329) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66205 HOMO: -6.56339 LUMO: -0.68573 factor:1 | 1 (-1.08805) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66343 HOMO: -6.31032 LUMO: -0.31837 factor:1 | 1 (-1.08944) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.27444 HOMO: -6.72938 LUMO: -0.45987 factor:1 | 1 (-1.70044) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.00163 HOMO: -6.59876 LUMO: -1.03131 factor:1 | -1 (0.57236) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.82645 HOMO: -7.29265 LUMO: 0.29660 factor:1 | -1 (0.74755) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.22489 HOMO: -6.42189 LUMO: -0.51157 factor:1 | -1 (1.34911) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96592 HOMO: -6.27767 LUMO: -0.52790 factor:1 | 1 (-0.39193) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60678 HOMO: -6.41644 LUMO: -0.44627 factor:1 | 1 (-1.03278) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51682 HOMO: -6.23413 LUMO: -0.52790 factor:1 | 1 (-0.94282) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.18400 HOMO: -6.63414 LUMO: -0.44082 factor:1 | 1 (-0.61000) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02876 HOMO: -7.03142 LUMO: 0.47076 factor:1 | 1 (-0.45476) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.91938 HOMO: -6.62053 LUMO: -0.14422 factor:1 | -1 (1.65462) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.02719 HOMO: -6.22324 LUMO: 1.96194 factor:1 | -1 (1.54680) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63678 HOMO: -6.17971 LUMO: 1.71704 factor:1 | 1 (-0.06278) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.58824 HOMO: -6.70761 LUMO: 1.68711 factor:1 | -1 (0.98576) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.63874 HOMO: -6.52801 LUMO: 1.56193 factor:1 | -1 (0.93526) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86238 HOMO: -6.55794 LUMO: 1.52384 factor:1 | 1 (-1.28838) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14683 HOMO: -6.47359 LUMO: 1.82316 factor:1 | 1 (-0.57283) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23403 HOMO: -6.65863 LUMO: 1.83133 factor:1 | 1 (-1.66003) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78640 HOMO: -6.46270 LUMO: 1.90208 factor:1 | 1 (-1.21240) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78599 HOMO: -6.41917 LUMO: 2.03269 factor:1 | 1 (-1.21200) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93166 HOMO: -6.48992 LUMO: 1.87486 factor:1 | 1 (-1.35766) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.23480 HOMO: -6.51985 LUMO: 1.69527 factor:1 | 1 (-0.66080) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78834 HOMO: -6.36202 LUMO: 2.05718 factor:1 | 1 (-0.21434) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.35466 HOMO: -5.96474 LUMO: 1.88575 factor:1 | -1 (1.21934) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.16790 HOMO: -6.56339 LUMO: 2.04630 factor:1 | -1 (1.40609) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.92752 HOMO: -6.43277 LUMO: 1.98371 factor:1 | -1 (1.64648) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.56601 HOMO: -6.53345 LUMO: 2.06262 factor:1 | -1 (1.00799) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77642 HOMO: -5.81779 LUMO: 2.11432 factor:1 | 1 (-0.20243) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38314 HOMO: -5.91848 LUMO: 1.86942 factor:1 | -1 (0.19086) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.37987 HOMO: -6.48447 LUMO: 1.70343 factor:1 | -1 (0.19413) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61979 HOMO: -6.29671 LUMO: -0.89525 factor:1 | 1 (-1.04579) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96350 HOMO: -6.63414 LUMO: -0.76192 factor:1 | 1 (-0.38950) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22498 HOMO: -6.56883 LUMO: -0.86260 factor:1 | 1 (-0.65098) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93776 HOMO: -6.93074 LUMO: -0.27483 factor:1 | 1 (-0.36376) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10168 HOMO: -6.85999 LUMO: -0.01905 factor:1 | 1 (-0.52768) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29870 HOMO: -6.26406 LUMO: 0.21769 factor:1 | -1 (0.27530) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64577 HOMO: -6.62325 LUMO: 0.31293 factor:1 | 1 (-1.07177) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89564 HOMO: -6.59604 LUMO: 0.19592 factor:1 | 1 (-0.32164) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85275 HOMO: -6.43277 LUMO: -0.27756 factor:1 | 1 (-0.27875) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97463 HOMO: -6.54978 LUMO: -0.46531 factor:1 | 1 (-0.40063) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44518 HOMO: -6.65046 LUMO: -0.15783 factor:1 | -1 (0.12882) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38249 HOMO: -7.28721 LUMO: 0.23946 factor:1 | -1 (0.19151) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.71056 HOMO: -6.71849 LUMO: -0.56600 factor:1 | 1 (-1.13657) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74978 HOMO: -6.85183 LUMO: -0.84355 factor:1 | 1 (-1.17578) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62986 HOMO: -6.53345 LUMO: -0.84627 factor:1 | 1 (-1.05586) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52665 HOMO: -6.60148 LUMO: -0.63130 factor:1 | -1 (0.04735) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52203 HOMO: -6.36202 LUMO: -0.60137 factor:1 | -1 (0.05197) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.27887 HOMO: -6.28855 LUMO: -0.52790 factor:1 | 1 (-1.70487) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.24750 HOMO: -7.07224 LUMO: 0.41906 factor:1 | 1 (-1.67350) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00856 HOMO: -6.36202 LUMO: -0.24218 factor:1 | 1 (-1.43456) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.95177 HOMO: -6.43549 LUMO: 0.14150 factor:1 | 1 (-1.37777) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55818 HOMO: -6.76747 LUMO: -0.40545 factor:1 | 1 (-0.98418) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.37289 HOMO: -6.15249 LUMO: -0.51157 factor:1 | 1 (-1.79889) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.14186 HOMO: -6.33753 LUMO: -0.02993 factor:1 | 1 (-1.56787) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.55014 HOMO: -6.49808 LUMO: -0.83811 factor:1 | 1 (-1.97615) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.25674 HOMO: -6.64502 LUMO: -0.46259 factor:1 | -1 (0.31726) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.15142 HOMO: -6.34570 LUMO: 0.22041 factor:1 | 1 (-1.57742) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.18879 HOMO: -6.63414 LUMO: -0.13606 factor:1 | -1 (0.38520) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.40798 HOMO: -6.59604 LUMO: -0.79729 factor:1 | -1 (0.16602) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97035 HOMO: -7.09401 LUMO: 0.31837 factor:1 | 1 (-1.39635) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19040 HOMO: -6.48719 LUMO: -0.31021 factor:1 | -1 (0.38360) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47579 HOMO: -7.11306 LUMO: 0.39729 factor:1 | -1 (0.09821) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.38083 HOMO: -6.95251 LUMO: 0.41089 factor:1 | 1 (-1.80684) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.44361 HOMO: -6.61509 LUMO: -0.41906 factor:1 | 1 (-1.86961) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.48345 HOMO: -6.25318 LUMO: -0.47348 factor:1 | 1 (-1.90945) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84246 HOMO: -6.77019 LUMO: -0.10340 factor:1 | 1 (-1.26846) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82290 HOMO: -6.54706 LUMO: -0.46259 factor:1 | 1 (-0.24890) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97364 HOMO: -6.34297 LUMO: -0.50341 factor:1 | 1 (-1.39964) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.13378 HOMO: -6.20692 LUMO: -0.51974 factor:1 | 1 (-1.55978) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.25983 HOMO: -7.03686 LUMO: 0.46804 factor:1 | 1 (-1.68583) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72113 HOMO: -6.47087 LUMO: 0.22585 factor:1 | 1 (-0.14713) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74276 HOMO: -6.41917 LUMO: 0.19320 factor:1 | 1 (-1.16876) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97933 HOMO: -6.61237 LUMO: -0.04354 factor:1 | 1 (-1.40533) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09888 HOMO: -6.56339 LUMO: 0.36735 factor:1 | 1 (-0.52488) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81101 HOMO: -6.54978 LUMO: 1.12655 factor:1 | 1 (-0.23701) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79183 HOMO: -6.43277 LUMO: 1.17553 factor:1 | 1 (-0.21783) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73547 HOMO: -6.29944 LUMO: 1.40955 factor:1 | 1 (-0.16147) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.56082 HOMO: -6.74842 LUMO: 0.74015 factor:1 | 1 (-0.98682) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44874 HOMO: -6.15522 LUMO: 1.94289 factor:1 | -1 (0.12525) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64420 HOMO: -6.20147 LUMO: 1.40139 factor:1 | 1 (-1.07020) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.19588 HOMO: -6.41100 LUMO: 1.40139 factor:1 | 1 (-1.62188) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69307 HOMO: -6.74570 LUMO: 1.80956 factor:1 | 1 (-1.11907) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41257 HOMO: -6.60148 LUMO: -1.04764 factor:1 | 1 (-0.83857) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62303 HOMO: -6.82734 LUMO: -0.83267 factor:1 | 1 (-1.04903) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90630 HOMO: -7.01782 LUMO: -0.32382 factor:1 | 1 (-0.33231) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92132 HOMO: -6.54434 LUMO: 0.11157 factor:1 | 1 (-0.34733) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.75404 HOMO: -6.53617 LUMO: 0.32926 factor:1 | 1 (-2.18004) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45720 HOMO: -6.62597 LUMO: -0.60137 factor:1 | 1 (-0.88320) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.74939 HOMO: -6.60965 LUMO: -0.75376 factor:1 | 1 (-2.17539) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.11773 HOMO: -6.29399 LUMO: 0.06803 factor:1 | 1 (-1.54373) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.52285 HOMO: -6.60692 LUMO: -0.47076 factor:1 | 1 (-1.94885) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.03464 HOMO: -7.33891 LUMO: 0.39184 factor:1 | 1 (-2.46064) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.95459 HOMO: -6.60692 LUMO: 1.46125 factor:1 | 1 (-2.38059) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.73806 HOMO: -6.21780 LUMO: 2.09256 factor:1 | 1 (-3.16406) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.10988 HOMO: -6.28311 LUMO: 1.80411 factor:1 | 1 (-2.53588) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.39512 HOMO: -6.51168 LUMO: 1.84765 factor:1 | 1 (-1.82112) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01424 HOMO: -6.66951 LUMO: 2.01636 factor:1 | 1 (-1.44024) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53799 HOMO: -6.75387 LUMO: 1.73881 factor:1 | 1 (-0.96399) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.07160 HOMO: -6.77291 LUMO: 1.89935 factor:1 | 1 (-1.49761) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.55077 HOMO: -6.36474 LUMO: 1.61091 factor:1 | 1 (-1.97677) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.21300 HOMO: -6.60420 LUMO: 1.40955 factor:1 | 1 (-1.63900) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.13694 HOMO: -6.81645 LUMO: 1.59731 factor:1 | 1 (-1.56294) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52158 HOMO: -5.90215 LUMO: 2.12249 factor:1 | 1 (-0.94758) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99455 HOMO: -6.26950 LUMO: 1.62996 factor:1 | 1 (-0.42055) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14100 HOMO: -6.41100 LUMO: 1.80684 factor:1 | 1 (-0.56700) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01376 HOMO: -6.64230 LUMO: 2.23405 factor:1 | 1 (-0.43976) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56932 HOMO: -6.66951 LUMO: 2.21501 factor:1 | -1 (0.00468) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43378 HOMO: -6.90897 LUMO: 2.00004 factor:1 | -1 (0.14022) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13126 HOMO: -6.61781 LUMO: 1.42043 factor:1 | 1 (-0.55726) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94694 HOMO: -6.56611 LUMO: 1.60003 factor:1 | -1 (0.62706) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.32851 HOMO: -6.70489 LUMO: 1.78779 factor:1 | 1 (-1.75451) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.99478 HOMO: -6.46815 LUMO: 1.59459 factor:1 | 1 (-2.42078) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.38924 HOMO: -6.31304 LUMO: 1.36873 factor:1 | 1 (-1.81524) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77285 HOMO: -6.22597 LUMO: 1.54833 factor:1 | 1 (-1.19885) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05050 HOMO: -5.63004 LUMO: 1.96466 factor:1 | 1 (-0.47650) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45111 HOMO: -7.02598 LUMO: 1.79323 factor:1 | -1 (0.12289) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05061 HOMO: -6.78924 LUMO: 2.10888 factor:1 | 1 (-0.47661) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84396 HOMO: -6.13345 LUMO: 2.07351 factor:1 | 1 (-0.26996) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.92675 HOMO: -6.46270 LUMO: -0.37552 factor:1 | -1 (0.64725) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.17475 HOMO: -6.51985 LUMO: -0.49525 factor:1 | -1 (0.39925) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.07630 HOMO: -6.60965 LUMO: 1.90480 factor:1 | -1 (0.49770) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.07348 HOMO: -6.51168 LUMO: 1.92112 factor:1 | 1 (-1.49948) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11118 HOMO: -6.71305 LUMO: 1.91024 factor:1 | 1 (-0.53718) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.02039 HOMO: -6.86815 LUMO: 2.02997 factor:1 | 1 (-1.44639) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01378 HOMO: -6.69944 LUMO: 1.95106 factor:1 | 1 (-1.43978) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42068 HOMO: -6.45182 LUMO: 1.66806 factor:1 | 1 (-0.84668) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95509 HOMO: -6.44638 LUMO: 2.16058 factor:1 | 1 (-0.38110) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24519 HOMO: -6.65591 LUMO: 1.95106 factor:1 | 1 (-0.67120) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99258 HOMO: -6.35114 LUMO: 1.42316 factor:1 | 1 (-1.41858) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.95190 HOMO: -6.48719 LUMO: 1.59187 factor:1 | 1 (-1.37790) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35826 HOMO: -7.05591 LUMO: 1.61908 factor:1 | 1 (-0.78426) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.32174 HOMO: -6.92258 LUMO: 1.87214 factor:1 | 1 (-0.74774) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80921 HOMO: -5.85861 LUMO: 2.11705 factor:1 | 1 (-1.23521) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.95794 HOMO: -6.27767 LUMO: 1.75513 factor:1 | 1 (-1.38394) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84726 HOMO: -6.16882 LUMO: 1.73881 factor:1 | 1 (-0.27326) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63432 HOMO: -6.62053 LUMO: 1.39594 factor:1 | 1 (-1.06032) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11899 HOMO: -5.46405 LUMO: 1.68166 factor:1 | 1 (-0.54499) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79587 HOMO: -6.39740 LUMO: 1.68711 factor:1 | 1 (-1.22187) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29333 HOMO: -6.99333 LUMO: 2.08439 factor:1 | 1 (-0.71933) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50306 HOMO: -6.16882 LUMO: 1.71976 factor:1 | -1 (0.07094) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14805 HOMO: -7.19741 LUMO: 2.24766 factor:1 | 1 (-0.57405) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24367 HOMO: -6.77291 LUMO: 2.17691 factor:1 | 1 (-0.66967) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22816 HOMO: -6.29944 LUMO: 2.16603 factor:1 | 1 (-0.65416) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89517 HOMO: -6.10079 LUMO: 1.83949 factor:1 | 1 (-1.32117) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93323 HOMO: -6.63686 LUMO: 2.05990 factor:1 | 1 (-1.35924) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24422 HOMO: -6.91713 LUMO: 1.87486 factor:1 | 1 (-0.67022) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31924 HOMO: -6.63958 LUMO: 1.79323 factor:1 | 1 (-0.74524) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76714 HOMO: -6.61781 LUMO: 1.70071 factor:1 | 1 (-1.19314) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.88216 HOMO: -6.20420 LUMO: 1.82861 factor:1 | 1 (-1.30816) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63132 HOMO: -6.47903 LUMO: -2.16875 factor:1 | 1 (-1.05733) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94241 HOMO: -6.53073 LUMO: 2.18235 factor:1 | 1 (-0.36841) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.37429 HOMO: -7.01782 LUMO: 1.72520 factor:1 | 1 (-0.80029) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82931 HOMO: -6.66135 LUMO: -0.75648 factor:1 | 1 (-1.25532) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60098 HOMO: -7.56749 LUMO: 0.22585 factor:1 | 1 (-1.02698) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16647 HOMO: -6.45182 LUMO: -0.71294 factor:1 | 1 (-0.59247) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95708 HOMO: -6.31032 LUMO: -0.34286 factor:1 | 1 (-0.38308) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50691 HOMO: -6.41917 LUMO: 2.04085 factor:1 | 1 (-0.93292) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93062 HOMO: -6.61781 LUMO: 1.98915 factor:1 | 1 (-1.35662) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44053 HOMO: -5.86405 LUMO: 1.57282 factor:1 | -1 (0.13347) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54583 HOMO: -6.44094 LUMO: 1.80956 factor:1 | 1 (-0.97183) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.76011 HOMO: -6.59060 LUMO: 2.08167 factor:1 | 1 (-2.18611) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.29550 HOMO: -6.20147 LUMO: 1.69799 factor:1 | 1 (-1.72150) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17376 HOMO: -6.50352 LUMO: -0.41361 factor:1 | 1 (-1.59976) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52036 HOMO: -6.10896 LUMO: -0.55783 factor:1 | 1 (-0.94636) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.79755 HOMO: -6.74842 LUMO: -0.56872 factor:1 | 1 (-2.22355) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.28818 HOMO: -6.59060 LUMO: -0.22041 factor:1 | 1 (-1.71418) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.00876 HOMO: -6.22052 LUMO: -0.60137 factor:1 | 1 (-2.43477) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.66461 HOMO: -6.65863 LUMO: 0.07891 factor:1 | 1 (-3.09061) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91590 HOMO: -6.57427 LUMO: 1.71160 factor:1 | 1 (-1.34190) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.53646 HOMO: -5.84773 LUMO: 1.99459 factor:1 | 1 (-1.96246) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.89391 HOMO: -6.02188 LUMO: 1.91296 factor:1 | 1 (-2.31991) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.89121 HOMO: -6.17698 LUMO: 2.00004 factor:1 | 1 (-2.31721) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83710 HOMO: -6.02732 LUMO: 1.90752 factor:1 | 1 (-1.26310) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.19229 HOMO: -6.68584 LUMO: -0.50885 factor:1 | 1 (-1.61829) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14519 HOMO: -6.61781 LUMO: -0.73471 factor:1 | 1 (-0.57119) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36792 HOMO: -6.66407 LUMO: -0.79729 factor:1 | 1 (-0.79392) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66733 HOMO: -6.56339 LUMO: 0.23130 factor:1 | 1 (-1.09333) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17501 HOMO: -6.76747 LUMO: 0.08980 factor:1 | 1 (-1.60101) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09295 HOMO: -6.70489 LUMO: -0.53334 factor:1 | 1 (-0.51895) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00859 HOMO: -7.28993 LUMO: 0.10885 factor:1 | 1 (-0.43459) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79859 HOMO: -6.22052 LUMO: 0.51974 factor:1 | 1 (-1.22459) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.88763 HOMO: -6.81645 LUMO: 0.25307 factor:1 | 1 (-1.31363) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.63989 HOMO: -6.80285 LUMO: 0.02721 factor:1 | 1 (-2.06589) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.65575 HOMO: -6.51441 LUMO: 0.08163 factor:1 | 1 (-2.08175) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.66895 HOMO: -6.73482 LUMO: -0.77008 factor:1 | 1 (-2.09495) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00929 HOMO: -6.29127 LUMO: -0.44355 factor:1 | 1 (-1.43529) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.56983 HOMO: -6.72938 LUMO: -0.64763 factor:1 | 1 (-0.99583) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90113 HOMO: -6.49264 LUMO: -0.74559 factor:1 | 1 (-1.32713) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.02167 HOMO: -6.67223 LUMO: -0.55239 factor:1 | 1 (-1.44767) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96799 HOMO: -6.33481 LUMO: 0.33198 factor:1 | 1 (-0.39399) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08876 HOMO: -6.76475 LUMO: -0.25307 factor:1 | 1 (-0.51476) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.46895 HOMO: -6.65318 LUMO: 0.03810 factor:1 | 1 (-0.89496) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.37848 HOMO: -6.09263 LUMO: 0.21497 factor:1 | 1 (-0.80448) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.10132 HOMO: -6.32120 LUMO: -0.85444 factor:1 | 1 (-1.52732) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12938 HOMO: -6.57155 LUMO: -0.67484 factor:1 | 1 (-0.55538) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89863 HOMO: -6.53345 LUMO: -0.78913 factor:1 | 1 (-0.32463) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13395 HOMO: -7.07768 LUMO: 0.28844 factor:1 | 1 (-0.55996) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69422 HOMO: -6.75114 LUMO: 0.18776 factor:1 | 1 (-0.12022) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.71247 HOMO: -6.77019 LUMO: -0.12245 factor:1 | 1 (-1.13847) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.49319 HOMO: -6.43549 LUMO: 0.16327 factor:1 | 1 (-1.91919) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.79733 HOMO: -6.69400 LUMO: -0.16327 factor:1 | 1 (-2.22333) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.11903 HOMO: -6.38651 LUMO: -0.61770 factor:1 | 1 (-1.54504) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.92150 HOMO: -6.34297 LUMO: -0.33198 factor:1 | 1 (-2.34750) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.09269 HOMO: -7.51578 LUMO: 0.02177 factor:1 | 1 (-1.51869) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.92748 HOMO: -6.47359 LUMO: -0.22585 factor:1 | 1 (-2.35349) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.96871 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-2.39471) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17740 HOMO: -6.75659 LUMO: -0.57688 factor:1 | 1 (-1.60340) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.77594 HOMO: -6.73754 LUMO: -0.61226 factor:1 | 1 (-2.20195) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52155 HOMO: -7.37429 LUMO: 0.31293 factor:1 | 1 (-0.94755) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.11612 HOMO: -6.23413 LUMO: -0.90886 factor:1 | 1 (-1.54212) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28359 HOMO: -6.51985 LUMO: -0.68028 factor:1 | 1 (-0.70959) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.19991 HOMO: -6.52257 LUMO: -0.77280 factor:1 | 1 (-1.62591) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93945 HOMO: -7.29537 LUMO: 0.31837 factor:1 | 1 (-0.36545) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91873 HOMO: -6.08447 LUMO: 0.25851 factor:1 | 1 (-1.34473) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19986 HOMO: -6.20964 LUMO: 0.13606 factor:1 | 1 (-0.62586) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01496 HOMO: -6.49808 LUMO: -0.14150 factor:1 | 1 (-0.44096) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.50429 HOMO: -7.10761 LUMO: 0.28028 factor:1 | 1 (-1.93029) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.92357 HOMO: -6.60965 LUMO: -0.62858 factor:1 | 1 (-2.34957) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.36402 HOMO: -6.40012 LUMO: -0.26939 factor:1 | 1 (-1.79002) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11069 HOMO: -6.65318 LUMO: -0.73199 factor:1 | 1 (-0.53669) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95613 HOMO: -6.51441 LUMO: -0.44899 factor:1 | 1 (-0.38213) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98492 HOMO: -6.28583 LUMO: -0.48708 factor:1 | 1 (-0.41092) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08647 HOMO: -6.96884 LUMO: 0.19864 factor:1 | 1 (-0.51247) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19442 HOMO: -6.89809 LUMO: 0.34558 factor:1 | 1 (-0.62042) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31243 HOMO: -6.67495 LUMO: -0.15510 factor:1 | 1 (-0.73844) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.05071 HOMO: -7.34980 LUMO: 0.19864 factor:1 | 1 (-1.47671) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09719 HOMO: -6.71305 LUMO: -0.81634 factor:1 | 1 (-0.52319) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.53806 HOMO: -6.39468 LUMO: -0.47076 factor:1 | 1 (-1.96406) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89642 HOMO: -6.31304 LUMO: 1.39594 factor:1 | 1 (-1.32242) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.12118 HOMO: -6.57155 LUMO: 1.55105 factor:1 | 1 (-1.54718) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.58702 HOMO: -6.68312 LUMO: 1.69255 factor:1 | 1 (-2.01302) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.20524 HOMO: -6.61509 LUMO: 1.73881 factor:1 | 1 (-1.63124) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.72411 HOMO: -6.17971 LUMO: 1.90208 factor:1 | 1 (-2.15011) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86842 HOMO: -6.53073 LUMO: 1.73337 factor:1 | 1 (-1.29442) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.96488 HOMO: -5.91303 LUMO: 1.90480 factor:1 | 1 (-1.39088) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.10546 HOMO: -6.42733 LUMO: 1.80139 factor:1 | 1 (-1.53146) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54270 HOMO: -6.78924 LUMO: 2.31569 factor:1 | 1 (-0.96870) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72539 HOMO: -6.04093 LUMO: 1.91568 factor:1 | 1 (-1.15140) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60278 HOMO: -6.90081 LUMO: 2.36739 factor:1 | 1 (-1.02878) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68093 HOMO: -6.60965 LUMO: 2.18507 factor:1 | 1 (-1.10693) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03235 HOMO: -6.75387 LUMO: 2.48712 factor:1 | 1 (-0.45835) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10936 HOMO: -6.56883 LUMO: 1.71432 factor:1 | 1 (-0.53536) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05052 HOMO: -6.41644 LUMO: 1.72792 factor:1 | 1 (-0.47653) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98486 HOMO: -6.92530 LUMO: 2.54426 factor:1 | 1 (-0.41086) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00152 HOMO: -6.41644 LUMO: 2.70209 factor:1 | 1 (-0.42752) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66905 HOMO: -6.29671 LUMO: 2.14698 factor:1 | 1 (-0.09505) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36095 HOMO: -6.29127 LUMO: 1.87486 factor:1 | 1 (-0.78695) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67718 HOMO: -6.75931 LUMO: 2.78917 factor:1 | 1 (-1.10318) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73582 HOMO: -6.40828 LUMO: 1.86942 factor:1 | 1 (-0.16183) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.18583 HOMO: -6.45726 LUMO: 1.97010 factor:1 | -1 (0.38817) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.21609 HOMO: -6.43277 LUMO: 1.22723 factor:1 | -1 (0.35791) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94764 HOMO: -6.63414 LUMO: 1.62452 factor:1 | 1 (-0.37364) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15462 HOMO: -6.54162 LUMO: 2.16058 factor:1 | -1 (0.41938) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.84473 HOMO: -6.40284 LUMO: 1.88575 factor:1 | -1 (0.72927) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93727 HOMO: -6.20964 LUMO: 1.84221 factor:1 | 1 (-0.36327) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90020 HOMO: -6.58516 LUMO: 1.69799 factor:1 | 1 (-1.32620) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91254 HOMO: -6.44094 LUMO: 2.05446 factor:1 | 1 (-0.33854) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.13171 HOMO: -6.61509 LUMO: 2.16058 factor:1 | 1 (-1.55772) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.82854 HOMO: -6.65591 LUMO: 1.69527 factor:1 | 1 (-2.25454) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.98202 HOMO: -5.55112 LUMO: 1.80411 factor:1 | 1 (-2.40802) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.10728 HOMO: -6.68312 LUMO: 2.38100 factor:1 | 1 (-1.53328) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.98588 HOMO: -6.51168 LUMO: 2.14698 factor:1 | -1 (0.58812) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.86264 HOMO: -6.04637 LUMO: 1.48302 factor:1 | -1 (0.71136) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.02879 HOMO: -6.81645 LUMO: -0.74287 factor:1 | -1 (0.54521) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64396 HOMO: -6.96884 LUMO: -0.97961 factor:1 | 1 (-0.06996) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68145 HOMO: -6.45998 LUMO: 0.09796 factor:1 | 1 (-1.10745) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54645 HOMO: -6.44638 LUMO: 0.09524 factor:1 | 1 (-0.97245) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63307 HOMO: -6.16338 LUMO: -0.54151 factor:1 | 1 (-0.05908) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67223 HOMO: -6.35930 LUMO: -0.47892 factor:1 | 1 (-0.09823) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65280 HOMO: -6.65318 LUMO: -0.00272 factor:1 | 1 (-0.07880) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75874 HOMO: -6.50080 LUMO: 0.14694 factor:1 | 1 (-0.18474) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47457 HOMO: -6.60420 LUMO: 0.94968 factor:1 | -1 (0.09943) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33994 HOMO: -6.60148 LUMO: -0.77552 factor:1 | 1 (-0.76595) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.10616 HOMO: -6.81645 LUMO: -1.05580 factor:1 | 1 (-1.53216) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17234 HOMO: -6.57971 LUMO: -0.82178 factor:1 | 1 (-1.59834) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23996 HOMO: -6.09263 LUMO: -0.45171 factor:1 | 1 (-1.66596) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.27207 HOMO: -6.74298 LUMO: -0.61770 factor:1 | 1 (-1.69807) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.32775 HOMO: -6.72393 LUMO: 1.21091 factor:1 | 1 (-1.75375) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.88825 HOMO: -6.30488 LUMO: 1.70071 factor:1 | 1 (-2.31425) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98220 HOMO: -6.38107 LUMO: 1.55649 factor:1 | 1 (-0.40820) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04886 HOMO: -6.17154 LUMO: 1.46669 factor:1 | 1 (-0.47487) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.72612 HOMO: -6.86543 LUMO: 1.98643 factor:1 | 1 (-2.15212) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.02189 HOMO: -6.69944 LUMO: 1.65173 factor:1 | 1 (-1.44789) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.62680 HOMO: -6.77836 LUMO: 2.16331 factor:1 | 1 (-2.05280) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94118 HOMO: -6.42189 LUMO: 2.36467 factor:1 | 1 (-1.36718) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.60816 HOMO: -7.00965 LUMO: 2.04358 factor:1 | 1 (-2.03416) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52232 HOMO: -6.36746 LUMO: 2.13881 factor:1 | 1 (-0.94832) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51532 HOMO: -6.37835 LUMO: 1.89935 factor:1 | 1 (-0.94132) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53657 HOMO: -7.03959 LUMO: 1.27349 factor:1 | 1 (-0.96258) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.10706 HOMO: -6.67495 LUMO: -0.89253 factor:1 | 1 (-1.53306) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14936 HOMO: -6.71849 LUMO: -0.97961 factor:1 | 1 (-0.57536) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.95849 HOMO: -6.47903 LUMO: 0.01633 factor:1 | 1 (-1.38449) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20272 HOMO: -6.38379 LUMO: 0.01088 factor:1 | 1 (-0.62872) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93446 HOMO: -6.49536 LUMO: -0.55239 factor:1 | 1 (-1.36046) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.27635 HOMO: -6.53345 LUMO: -0.53879 factor:1 | 1 (-0.70235) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90423 HOMO: -6.16610 LUMO: 2.15514 factor:1 | 1 (-1.33023) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08797 HOMO: -6.35114 LUMO: 1.98643 factor:1 | 1 (-0.51397) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66918 HOMO: -6.43277 LUMO: 2.16058 factor:1 | 1 (-1.09518) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87506 HOMO: -6.89809 LUMO: 2.20684 factor:1 | 1 (-1.30106) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54311 HOMO: -6.54434 LUMO: 1.93473 factor:1 | -1 (0.03088) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08397 HOMO: -6.72938 LUMO: 2.03269 factor:1 | 1 (-0.50997) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60521 HOMO: -6.90353 LUMO: 2.19868 factor:1 | 1 (-0.03121) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47226 HOMO: -6.41372 LUMO: 2.02453 factor:1 | -1 (0.10174) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91967 HOMO: -6.46543 LUMO: 1.90752 factor:1 | 1 (-0.34567) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.30173 HOMO: -6.55522 LUMO: 2.11977 factor:1 | 1 (-1.72773) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39954 HOMO: -6.28855 LUMO: 2.02181 factor:1 | 1 (-0.82554) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98184 HOMO: -6.45726 LUMO: 1.52112 factor:1 | 1 (-0.40784) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81077 HOMO: -6.37291 LUMO: 2.11705 factor:1 | -1 (0.76322) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89584 HOMO: -6.88448 LUMO: 2.24494 factor:1 | -1 (0.67816) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.57365 HOMO: -6.86271 LUMO: 2.41637 factor:1 | -1 (1.00034) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94457 HOMO: -6.69400 LUMO: 2.34562 factor:1 | -1 (0.62943) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.54587 HOMO: -6.18243 LUMO: 2.53882 factor:1 | -1 (1.02813) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79397 HOMO: -6.61237 LUMO: 2.54154 factor:1 | 1 (-1.21997) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93036 HOMO: -6.69672 LUMO: 2.16331 factor:1 | 1 (-0.35636) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02108 HOMO: -6.33481 LUMO: 2.34018 factor:1 | 1 (-0.44708) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63343 HOMO: -5.99739 LUMO: 2.37283 factor:1 | 1 (-0.05943) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16242 HOMO: -6.49808 LUMO: 2.47351 factor:1 | 1 (-0.58842) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29418 HOMO: -6.22052 LUMO: 1.86398 factor:1 | 1 (-0.72018) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50801 HOMO: -6.32665 LUMO: 2.28031 factor:1 | -1 (0.06599) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59250 HOMO: -5.98378 LUMO: 2.16331 factor:1 | 1 (-0.01850) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90331 HOMO: -6.08991 LUMO: 2.30208 factor:1 | 1 (-0.32931) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19026 HOMO: -7.07224 LUMO: 1.55105 factor:1 | 1 (-0.61626) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61737 HOMO: -6.84638 LUMO: 1.76874 factor:1 | 1 (-0.04337) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.99578 HOMO: -6.68856 LUMO: 1.47758 factor:1 | -1 (0.57821) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05127 HOMO: -6.69672 LUMO: 1.71976 factor:1 | -1 (0.52273) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.00938 HOMO: -6.86543 LUMO: 2.24766 factor:1 | -1 (2.56462) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.03033 HOMO: -7.21646 LUMO: 1.71976 factor:1 | -1 (2.54367) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.31091 HOMO: -6.94162 LUMO: 2.21773 factor:1 | -1 (2.26309) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.65326 HOMO: -6.34842 LUMO: 2.04358 factor:1 | -1 (2.92073) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.99025 HOMO: -6.53345 LUMO: 1.96738 factor:1 | -1 (2.58375) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.01498 HOMO: -6.34842 LUMO: 1.88303 factor:1 | -1 (1.55902) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.07299 HOMO: -6.38651 LUMO: 2.08983 factor:1 | -1 (1.50101) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.71513 HOMO: -6.01372 LUMO: 1.43676 factor:1 | -1 (1.85886) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.86564 HOMO: -6.30216 LUMO: 1.41771 factor:1 | -1 (1.70836) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.87138 HOMO: -6.52801 LUMO: 1.77146 factor:1 | -1 (1.70262) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97526 HOMO: -6.53617 LUMO: 1.72792 factor:1 | 1 (-0.40126) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43710 HOMO: -6.56611 LUMO: 2.20412 factor:1 | -1 (0.13690) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02674 HOMO: -6.66679 LUMO: -0.72927 factor:1 | 1 (-0.45274) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00960 HOMO: -6.85455 LUMO: -0.85444 factor:1 | 1 (-0.43560) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44287 HOMO: -7.21646 LUMO: 0.27211 factor:1 | -1 (0.13113) | 1 | 1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16699 HOMO: -6.57971 LUMO: -0.41361 factor:1 | 1 (-0.59299) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.36034 HOMO: -7.03142 LUMO: -1.14288 factor:1 | -1 (0.21366) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93899 HOMO: -6.29944 LUMO: 0.06803 factor:1 | 1 (-0.36499) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.04626 HOMO: -6.47359 LUMO: 0.28028 factor:1 | -1 (0.52774) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44404 HOMO: -6.42189 LUMO: 1.61364 factor:1 | -1 (0.12996) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.41729 HOMO: -6.41100 LUMO: 1.80956 factor:1 | -1 (0.15671) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10500 HOMO: -6.83278 LUMO: 1.83949 factor:1 | 1 (-0.53100) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05108 HOMO: -6.78380 LUMO: -0.76192 factor:1 | -1 (0.52292) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02633 HOMO: -6.95795 LUMO: 2.13609 factor:1 | 1 (-0.45233) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81278 HOMO: -6.57155 LUMO: 1.89119 factor:1 | 1 (-0.23878) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.58554 HOMO: -6.65591 LUMO: 1.93745 factor:1 | 1 (-0.01154) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.72455 HOMO: -6.44638 LUMO: 2.26943 factor:1 | -1 (1.84945) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.65873 HOMO: -5.88038 LUMO: 1.90480 factor:1 | -1 (1.91527) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.75263 HOMO: -6.22052 LUMO: 2.17691 factor:1 | -1 (1.82137) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10878 HOMO: -6.04637 LUMO: 2.23950 factor:1 | 1 (-0.53479) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84600 HOMO: -6.44366 LUMO: 2.24766 factor:1 | 1 (-0.27201) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.16396 HOMO: -6.81917 LUMO: 2.08439 factor:1 | 1 (-1.58996) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.27752 HOMO: -6.48447 LUMO: 2.28576 factor:1 | 1 (-0.70352) | -1 | -1 |
| G: -5684.20830 HOMO: -7.07224 LUMO: -0.58232 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08698 HOMO: -6.54434 LUMO: 1.99187 factor:1 | 1 (-1.51298) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67220 HOMO: -6.17698 LUMO: -0.65852 factor:1 | 1 (-1.09820) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.95626 HOMO: -6.08174 LUMO: -0.58504 factor:1 | 1 (-1.38226) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19894 HOMO: -6.55250 LUMO: -0.86804 factor:1 | 1 (-0.62494) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35605 HOMO: -6.57699 LUMO: -0.89525 factor:1 | 1 (-0.78206) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87722 HOMO: -6.63141 LUMO: -1.04220 factor:1 | 1 (-0.30322) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09270 HOMO: -6.69128 LUMO: -0.76736 factor:1 | 1 (-0.51870) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.75685 HOMO: -6.25318 LUMO: -1.03131 factor:1 | 1 (-1.18285) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.75622 HOMO: -6.69944 LUMO: 0.01905 factor:1 | 1 (-1.18223) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02084 HOMO: -6.28583 LUMO: 0.38368 factor:1 | 1 (-0.44684) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19523 HOMO: -6.90081 LUMO: -0.83811 factor:1 | 1 (-0.62124) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.82175 HOMO: -6.78380 LUMO: -0.10068 factor:1 | -1 (1.75225) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.91181 HOMO: -6.30488 LUMO: -0.98505 factor:1 | -1 (0.66219) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05004 HOMO: -6.29671 LUMO: -1.79051 factor:1 | -1 (0.52396) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.55727 HOMO: -6.76747 LUMO: -0.22041 factor:1 | -1 (1.01673) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59484 HOMO: -6.22597 LUMO: -0.94968 factor:1 | 1 (-0.02084) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.55286 HOMO: -6.73482 LUMO: 0.05987 factor:1 | -1 (1.02113) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82655 HOMO: -6.28855 LUMO: 0.34831 factor:1 | 1 (-0.25255) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75642 HOMO: -6.69400 LUMO: 0.25307 factor:1 | 1 (-0.18243) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70690 HOMO: -6.70216 LUMO: 0.61226 factor:1 | 1 (-0.13290) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11412 HOMO: -6.70216 LUMO: 0.17415 factor:1 | 1 (-0.54012) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84023 HOMO: -6.70761 LUMO: 0.24762 factor:1 | 1 (-1.26623) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97324 HOMO: -6.68856 LUMO: -0.84900 factor:1 | 1 (-0.39925) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90020 HOMO: -6.71033 LUMO: -0.38640 factor:1 | 1 (-1.32620) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16693 HOMO: -6.24501 LUMO: -0.09252 factor:1 | 1 (-0.59294) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91177 HOMO: -6.81645 LUMO: -0.07347 factor:1 | 1 (-0.33777) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31646 HOMO: -6.49536 LUMO: 0.09796 factor:1 | 1 (-0.74246) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.46246 HOMO: -6.71033 LUMO: -0.26395 factor:1 | -1 (0.11154) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.88578 HOMO: -6.70489 LUMO: -0.09252 factor:1 | 1 (-1.31178) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15771 HOMO: -6.23685 LUMO: 0.39729 factor:1 | 1 (-0.58371) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93411 HOMO: -6.69400 LUMO: -0.05442 factor:1 | 1 (-0.36012) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84062 HOMO: -6.36202 LUMO: 0.09796 factor:1 | 1 (-0.26662) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.34560 HOMO: -6.54978 LUMO: 0.15510 factor:1 | 1 (-1.77160) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62049 HOMO: -6.77836 LUMO: 0.25851 factor:1 | 1 (-1.04650) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15023 HOMO: -5.70623 LUMO: 0.73471 factor:1 | 1 (-0.57623) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00990 HOMO: -5.58378 LUMO: 0.89253 factor:1 | 1 (-0.43590) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29154 HOMO: -5.68718 LUMO: 0.87893 factor:1 | -1 (0.28245) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.93635 HOMO: -5.10486 LUMO: 1.11567 factor:1 | -1 (0.63764) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.18806 HOMO: -4.59328 LUMO: 1.27621 factor:1 | -1 (0.38594) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35944 HOMO: -4.45450 LUMO: 1.82044 factor:1 | -1 (0.21456) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.75951 HOMO: -4.64226 LUMO: 1.70615 factor:1 | -1 (0.81449) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38970 HOMO: -5.04227 LUMO: 1.04492 factor:1 | -1 (0.18430) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56211 HOMO: -4.85723 LUMO: 0.93607 factor:1 | -1 (0.01189) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54599 HOMO: -4.72934 LUMO: 1.00410 factor:1 | 1 (-0.97199) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.24244 HOMO: -4.56335 LUMO: 1.56738 factor:1 | 1 (-1.66844) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83378 HOMO: -5.48854 LUMO: 0.33198 factor:1 | 1 (-1.25978) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.40672 HOMO: -4.97424 LUMO: 1.33608 factor:1 | 1 (-0.83272) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02900 HOMO: -4.60145 LUMO: 1.74697 factor:1 | 1 (-0.45500) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77281 HOMO: -5.60010 LUMO: 0.74831 factor:1 | 1 (-0.19881) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85887 HOMO: -5.66541 LUMO: 0.66668 factor:1 | 1 (-0.28488) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79498 HOMO: -6.50080 LUMO: 0.07075 factor:1 | 1 (-0.22098) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69394 HOMO: -5.79603 LUMO: 0.22313 factor:1 | 1 (-1.11994) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.46523 HOMO: -4.68036 LUMO: 1.29798 factor:1 | -1 (0.10876) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76908 HOMO: -4.84363 LUMO: 1.34424 factor:1 | 1 (-0.19508) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.31277 HOMO: -4.62321 LUMO: 1.82861 factor:1 | -1 (0.26123) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.92435 HOMO: -5.83684 LUMO: 0.82178 factor:1 | -1 (0.64964) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05878 HOMO: -5.27629 LUMO: 0.57960 factor:1 | -1 (0.51522) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.57531 HOMO: -5.15928 LUMO: -2.96876 factor:1 | -1 (0.99869) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.90220 HOMO: -5.08853 LUMO: 0.89253 factor:1 | -1 (0.67179) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96280 HOMO: -6.42461 LUMO: 0.04354 factor:1 | 1 (-0.38880) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15719 HOMO: -6.42733 LUMO: -0.00544 factor:1 | 1 (-0.58319) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00250 HOMO: -5.87494 LUMO: 0.69933 factor:1 | 1 (-0.42850) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48896 HOMO: -5.07492 LUMO: 1.02587 factor:1 | -1 (0.08504) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16163 HOMO: -4.44362 LUMO: 1.99187 factor:1 | 1 (-0.58763) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76059 HOMO: -5.82052 LUMO: 0.43810 factor:1 | 1 (-0.18659) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43514 HOMO: -5.75793 LUMO: 0.76464 factor:1 | -1 (0.13886) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05814 HOMO: -5.09669 LUMO: 0.72382 factor:1 | 1 (-0.48414) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.79856 HOMO: -6.75387 LUMO: -2.02453 factor:1 | -1 (0.77544) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.83151 HOMO: -5.02322 LUMO: 1.14832 factor:1 | -1 (0.74249) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15595 HOMO: -5.75521 LUMO: 0.73471 factor:1 | -1 (0.41805) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.87529 HOMO: -5.89943 LUMO: 0.54967 factor:1 | -1 (0.69871) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.52467 HOMO: -5.80147 LUMO: 0.72382 factor:1 | -1 (1.04933) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15930 HOMO: -6.16066 LUMO: 0.39457 factor:1 | -1 (0.41470) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.85355 HOMO: -5.98650 LUMO: 0.76736 factor:1 | -1 (0.72045) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.62767 HOMO: -4.74839 LUMO: 1.88847 factor:1 | -1 (0.94633) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80206 HOMO: -5.62459 LUMO: 0.26939 factor:1 | 1 (-0.22806) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74807 HOMO: -4.88172 LUMO: 1.30070 factor:1 | 1 (-0.17407) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74802 HOMO: -5.09397 LUMO: 0.98505 factor:1 | 1 (-0.17402) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95673 HOMO: -6.50080 LUMO: -0.28300 factor:1 | 1 (-0.38273) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.10447 HOMO: -5.04227 LUMO: 1.49935 factor:1 | -1 (0.46953) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06133 HOMO: -5.22731 LUMO: 0.88437 factor:1 | 1 (-0.48733) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35051 HOMO: -4.95519 LUMO: 1.25717 factor:1 | -1 (0.22349) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15620 HOMO: -4.61233 LUMO: 1.27621 factor:1 | -1 (0.41780) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65049 HOMO: -4.70757 LUMO: 1.63813 factor:1 | 1 (-0.07649) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.71284 HOMO: -4.85179 LUMO: 1.11839 factor:1 | -1 (0.86116) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99746 HOMO: -4.97696 LUMO: 1.00138 factor:1 | 1 (-0.42346) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.33367 HOMO: -5.64636 LUMO: 0.81090 factor:1 | -1 (0.24033) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.09549 HOMO: -4.37831 LUMO: 1.90208 factor:1 | -1 (0.47851) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09899 HOMO: -4.67764 LUMO: 1.54561 factor:1 | 1 (-0.52499) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76731 HOMO: -5.87766 LUMO: 0.42994 factor:1 | 1 (-0.19331) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78130 HOMO: -6.03821 LUMO: 0.32382 factor:1 | 1 (-0.20730) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26994 HOMO: -5.99739 LUMO: 0.69389 factor:1 | -1 (0.30406) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35385 HOMO: -6.43821 LUMO: 0.15238 factor:1 | 1 (-0.77985) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.75152 HOMO: -6.63414 LUMO: -0.07347 factor:1 | 1 (-1.17752) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44132 HOMO: -6.50080 LUMO: 0.10068 factor:1 | -1 (0.13268) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92837 HOMO: -6.49264 LUMO: 0.19592 factor:1 | 1 (-0.35437) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54978 HOMO: -5.83956 LUMO: 0.12517 factor:1 | -1 (0.02422) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44855 HOMO: -6.50896 LUMO: 0.19048 factor:1 | -1 (0.12544) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.33051 HOMO: -6.56611 LUMO: 0.04898 factor:1 | -1 (0.24349) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48804 HOMO: -6.68040 LUMO: -0.08436 factor:1 | -1 (0.08596) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.41174 HOMO: -6.73754 LUMO: -0.08708 factor:1 | -1 (0.16226) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.65069 HOMO: -6.80285 LUMO: -0.10612 factor:1 | -1 (0.92331) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.23845 HOMO: -6.35658 LUMO: 0.02177 factor:1 | 1 (-0.66445) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65332 HOMO: -5.74160 LUMO: 0.14694 factor:1 | 1 (-0.07932) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30563 HOMO: -4.78376 LUMO: 0.92791 factor:1 | 1 (-0.73163) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14329 HOMO: -5.90215 LUMO: 0.36463 factor:1 | 1 (-0.56929) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64252 HOMO: -4.99329 LUMO: 0.85988 factor:1 | 1 (-0.06852) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12234 HOMO: -4.93887 LUMO: 1.33608 factor:1 | 1 (-0.54834) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.23189 HOMO: -5.19193 LUMO: 0.50341 factor:1 | 1 (-0.65789) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60118 HOMO: -6.64502 LUMO: -1.98643 factor:1 | 1 (-0.02718) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.09127 HOMO: -5.15384 LUMO: 0.94968 factor:1 | -1 (0.48273) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.76387 HOMO: -6.31032 LUMO: 0.08436 factor:1 | -1 (1.81013) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.25117 HOMO: -4.88716 LUMO: 0.82995 factor:1 | -1 (1.32283) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.55042 HOMO: -5.57017 LUMO: 0.19320 factor:1 | -1 (2.02357) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.53129 HOMO: -4.92254 LUMO: 0.93879 factor:1 | -1 (2.04270) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.83432 HOMO: -4.77288 LUMO: 1.60003 factor:1 | -1 (1.73968) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12693 HOMO: -4.97696 LUMO: 0.89798 factor:1 | 1 (-0.55294) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75980 HOMO: -5.00690 LUMO: 1.14288 factor:1 | 1 (-0.18580) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19627 HOMO: -4.88444 LUMO: 1.48574 factor:1 | 1 (-0.62227) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89041 HOMO: -5.03955 LUMO: 1.51023 factor:1 | 1 (-0.31641) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.07494 HOMO: -5.22459 LUMO: 0.99049 factor:1 | -1 (0.49906) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.36918 HOMO: -5.29534 LUMO: 0.96056 factor:1 | -1 (0.20482) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.90283 HOMO: -5.35520 LUMO: 0.68301 factor:1 | -1 (0.67117) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69327 HOMO: -5.27357 LUMO: 1.18642 factor:1 | 1 (-0.11927) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.21348 HOMO: -5.79875 LUMO: 0.61770 factor:1 | -1 (0.36052) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19488 HOMO: -7.64640 LUMO: -2.45175 factor:1 | 1 (-0.62088) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.26158 HOMO: -7.46953 LUMO: -1.29798 factor:1 | 1 (-0.68758) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80025 HOMO: -7.95389 LUMO: -0.37280 factor:1 | 1 (-1.22625) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76605 HOMO: -7.23279 LUMO: -1.19186 factor:1 | 1 (-1.19205) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.59355 HOMO: -7.14299 LUMO: -1.12927 factor:1 | -1 (0.98045) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22857 HOMO: -6.93074 LUMO: 0.31565 factor:1 | 1 (-0.65457) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.24795 HOMO: -6.63141 LUMO: 0.28028 factor:1 | -1 (0.32605) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02952 HOMO: -7.10489 LUMO: -1.07213 factor:1 | 1 (-0.45552) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72589 HOMO: -7.00693 LUMO: -0.69389 factor:1 | 1 (-0.15189) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28215 HOMO: -8.50356 LUMO: -1.79595 factor:1 | 1 (-0.70815) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05610 HOMO: -7.79334 LUMO: -2.33746 factor:1 | 1 (-0.48210) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01354 HOMO: -7.24367 LUMO: -0.85172 factor:1 | 1 (-0.43955) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43367 HOMO: -7.94028 LUMO: -0.20136 factor:1 | -1 (0.14033) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16838 HOMO: -7.22462 LUMO: 0.84627 factor:1 | 1 (-0.59438) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10201 HOMO: -6.54978 LUMO: 0.34831 factor:1 | 1 (-0.52801) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10783 HOMO: -6.86815 LUMO: 0.32109 factor:1 | 1 (-0.53383) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.20170 HOMO: -7.17564 LUMO: -1.28438 factor:1 | -1 (1.37230) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15700 HOMO: -7.03142 LUMO: -1.12655 factor:1 | 1 (-0.58300) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.87285 HOMO: -7.39878 LUMO: 0.15783 factor:1 | -1 (1.70115) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.00586 HOMO: -7.25728 LUMO: 0.42178 factor:1 | -1 (1.56814) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.06151 HOMO: -6.86543 LUMO: 0.93879 factor:1 | -1 (1.51249) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35291 HOMO: -7.09673 LUMO: -0.69661 factor:1 | -1 (0.22109) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.09217 HOMO: -7.74708 LUMO: 0.01088 factor:1 | -1 (0.48183) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.08219 HOMO: -6.80557 LUMO: 0.46531 factor:1 | -1 (1.49181) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.12260 HOMO: -7.29265 LUMO: 1.31975 factor:1 | -1 (1.45140) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.72424 HOMO: -6.93618 LUMO: 0.29388 factor:1 | -1 (0.84976) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89725 HOMO: -6.53073 LUMO: 0.71022 factor:1 | -1 (0.67675) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.72764 HOMO: -6.41917 LUMO: -1.24084 factor:1 | -1 (0.84636) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.82490 HOMO: -6.67495 LUMO: -1.09118 factor:1 | -1 (0.74910) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06809 HOMO: -6.97156 LUMO: -0.53606 factor:1 | 1 (-1.49410) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73222 HOMO: -6.85183 LUMO: -0.45715 factor:1 | 1 (-1.15823) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72439 HOMO: -7.12666 LUMO: -0.67484 factor:1 | 1 (-1.15039) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80929 HOMO: -7.49946 LUMO: -0.14694 factor:1 | 1 (-1.23529) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15213 HOMO: -7.44231 LUMO: 0.58232 factor:1 | 1 (-0.57813) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02149 HOMO: -7.36340 LUMO: -0.68301 factor:1 | 1 (-0.44749) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.77592 HOMO: -6.13073 LUMO: -0.54967 factor:1 | -1 (0.79808) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.07168 HOMO: -7.81511 LUMO: -0.06531 factor:1 | -1 (0.50232) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38023 HOMO: -7.26816 LUMO: -1.02587 factor:1 | -1 (0.19377) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.04496 HOMO: -7.98110 LUMO: -0.17960 factor:1 | -1 (0.52904) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71022 HOMO: -7.44776 LUMO: -1.00954 factor:1 | 1 (-0.13622) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.87219 HOMO: -7.47769 LUMO: -1.02859 factor:1 | -1 (0.70181) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94520 HOMO: -6.75659 LUMO: 0.39457 factor:1 | -1 (0.62880) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.96631 HOMO: -6.71849 LUMO: 0.36735 factor:1 | -1 (0.60768) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.00319 HOMO: -7.64096 LUMO: -1.43948 factor:1 | -1 (0.57081) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.69409 HOMO: -7.83144 LUMO: -1.36601 factor:1 | -1 (0.87991) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.23133 HOMO: -7.19469 LUMO: 0.35103 factor:1 | -1 (0.34267) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02832 HOMO: -7.03414 LUMO: 0.20409 factor:1 | 1 (-0.45432) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90209 HOMO: -7.22734 LUMO: 0.31293 factor:1 | 1 (-0.32809) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24544 HOMO: -6.93618 LUMO: 0.56055 factor:1 | 1 (-0.67144) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59351 HOMO: -6.94707 LUMO: -0.88709 factor:1 | 1 (-0.01951) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19858 HOMO: -6.86543 LUMO: -0.83267 factor:1 | 1 (-0.62458) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.08071 HOMO: -6.82189 LUMO: -1.15376 factor:1 | -1 (0.49329) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.42820 HOMO: -6.65046 LUMO: -0.46531 factor:1 | -1 (0.14580) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20775 HOMO: -6.52529 LUMO: 0.20953 factor:1 | 1 (-0.63375) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61147 HOMO: -6.80557 LUMO: 0.44355 factor:1 | 1 (-0.03747) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.15179 HOMO: -6.93074 LUMO: -0.81634 factor:1 | -1 (3.42221) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11944.10385 HOMO: -7.43143 LUMO: -0.45987 factor:1 | -1 (4.47015) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11944.66465 HOMO: -7.07224 LUMO: -0.68028 factor:1 | -1 (3.90935) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.22189 HOMO: -6.68040 LUMO: -0.71566 factor:1 | -1 (1.35211) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.21766 HOMO: -6.26406 LUMO: -1.09934 factor:1 | -1 (2.35634) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.15066 HOMO: -5.94569 LUMO: -0.72110 factor:1 | -1 (2.42334) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.03606 HOMO: -6.12256 LUMO: -0.42178 factor:1 | -1 (3.53794) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.07929 HOMO: -6.09807 LUMO: 0.11429 factor:1 | -1 (3.49470) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.83174 HOMO: -7.35252 LUMO: -0.55783 factor:1 | -1 (1.74226) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.73973 HOMO: -7.57837 LUMO: -0.76736 factor:1 | -1 (1.83427) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.32050 HOMO: -6.16066 LUMO: 0.01905 factor:1 | -1 (0.25350) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.32597 HOMO: -6.13345 LUMO: -0.41906 factor:1 | -1 (0.24803) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65245 HOMO: -6.10351 LUMO: -0.33742 factor:1 | 1 (-0.07845) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77833 HOMO: -7.24639 LUMO: -0.51702 factor:1 | 1 (-0.20433) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.27352 HOMO: -6.98244 LUMO: -1.82044 factor:1 | 1 (-0.69952) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61351 HOMO: -6.37563 LUMO: -1.67622 factor:1 | 1 (-0.03951) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.27927 HOMO: -5.79058 LUMO: -2.55243 factor:1 | -1 (0.29473) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13564 HOMO: -6.34025 LUMO: -0.27483 factor:1 | 1 (-0.56164) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56328 HOMO: -6.05453 LUMO: -0.51157 factor:1 | -1 (0.01072) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11989 HOMO: -7.53755 LUMO: -0.38912 factor:1 | 1 (-0.54589) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63215 HOMO: -7.00421 LUMO: -0.50885 factor:1 | 1 (-0.05815) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.04961 HOMO: -7.52123 LUMO: -0.37552 factor:1 | -1 (0.52439) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02097 HOMO: -6.70489 LUMO: -1.04764 factor:1 | 1 (-0.44697) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.92272 HOMO: -7.06408 LUMO: -1.16737 factor:1 | -1 (0.65128) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10089 HOMO: -6.71849 LUMO: -1.02315 factor:1 | 1 (-0.52689) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57101 HOMO: -6.16610 LUMO: -0.50885 factor:1 | -1 (0.00299) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.62022 HOMO: -6.48447 LUMO: 0.07619 factor:1 | -1 (1.95378) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.01072 HOMO: -7.06135 LUMO: 0.09796 factor:1 | -1 (0.56328) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.32216 HOMO: -6.47359 LUMO: 0.22585 factor:1 | -1 (0.25184) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.61306 HOMO: -6.10896 LUMO: -0.62314 factor:1 | -1 (0.96094) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.80860 HOMO: -6.88176 LUMO: -0.96600 factor:1 | -1 (0.76540) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.98784 HOMO: -6.67495 LUMO: 0.21769 factor:1 | -1 (0.58616) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69631 HOMO: -6.84911 LUMO: 0.38368 factor:1 | 1 (-0.12232) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.74949 HOMO: -6.83550 LUMO: 1.29798 factor:1 | -1 (0.82450) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.46725 HOMO: -6.67495 LUMO: 1.46941 factor:1 | -1 (0.10675) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.56927 HOMO: -6.81917 LUMO: 1.30887 factor:1 | -1 (1.00473) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.00953 HOMO: -6.56611 LUMO: 0.66396 factor:1 | -1 (0.56447) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75109 HOMO: -6.76203 LUMO: 0.60137 factor:1 | 1 (-0.17709) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.91638 HOMO: -6.55794 LUMO: 0.34286 factor:1 | -1 (0.65762) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.51896 HOMO: -6.83550 LUMO: 0.35919 factor:1 | -1 (1.05504) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.62995 HOMO: -7.17836 LUMO: 0.63130 factor:1 | -1 (0.94404) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56450 HOMO: -6.29944 LUMO: -0.69389 factor:1 | -1 (0.00950) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47495 HOMO: -7.06680 LUMO: -0.95784 factor:1 | -1 (0.09905) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91245 HOMO: -6.84638 LUMO: -0.87076 factor:1 | 1 (-0.33846) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07099 HOMO: -6.96339 LUMO: -1.05308 factor:1 | 1 (-0.49699) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.95538 HOMO: -6.75387 LUMO: -1.04220 factor:1 | -1 (0.61862) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.83867 HOMO: -6.71849 LUMO: -0.84355 factor:1 | -1 (0.73533) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.72329 HOMO: -7.16748 LUMO: 0.51702 factor:1 | -1 (0.85071) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.61565 HOMO: -6.92530 LUMO: 0.71566 factor:1 | -1 (1.95835) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13772 HOMO: -7.11034 LUMO: 0.01905 factor:1 | -1 (0.43628) | 1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50352 HOMO: -6.79468 LUMO: 0.77008 factor:1 | -1 (0.07048) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87969 HOMO: -6.52801 LUMO: 0.98233 factor:1 | 1 (-0.30569) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89365 HOMO: -6.76475 LUMO: 0.53334 factor:1 | 1 (-0.31965) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64393 HOMO: -5.29261 LUMO: 0.57416 factor:1 | 1 (-0.06993) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96631 HOMO: -6.57971 LUMO: 0.12789 factor:1 | 1 (-0.39231) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.79141 HOMO: -6.99333 LUMO: 0.51430 factor:1 | -1 (1.78259) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82537 HOMO: -6.41917 LUMO: 0.19048 factor:1 | 1 (-1.25137) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53630 HOMO: -6.16066 LUMO: 1.77146 factor:1 | 1 (-0.96230) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81604 HOMO: -6.90353 LUMO: 1.65717 factor:1 | 1 (-0.24205) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76920 HOMO: -5.94569 LUMO: 1.29526 factor:1 | 1 (-1.19521) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01159 HOMO: -6.60420 LUMO: 1.33880 factor:1 | 1 (-0.43759) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84897 HOMO: -6.23957 LUMO: 0.09524 factor:1 | 1 (-0.27497) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49641 HOMO: -6.80013 LUMO: 1.34696 factor:1 | 1 (-0.92241) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87323 HOMO: -7.53483 LUMO: -1.52384 factor:1 | 1 (-1.29923) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13502 HOMO: -7.62463 LUMO: -1.65717 factor:1 | 1 (-0.56102) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99654 HOMO: -7.62463 LUMO: -1.61364 factor:1 | 1 (-0.42254) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55497 HOMO: -8.04096 LUMO: -1.66806 factor:1 | 1 (-0.98097) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.70016 HOMO: -7.18381 LUMO: -1.17553 factor:1 | -1 (0.87384) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.68176 HOMO: -7.69538 LUMO: -1.36601 factor:1 | -1 (0.89223) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.30611 HOMO: -7.95117 LUMO: -1.48302 factor:1 | -1 (1.26789) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.24539 HOMO: -6.98516 LUMO: 0.35919 factor:1 | -1 (0.32860) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.26772 HOMO: -7.91579 LUMO: -0.32109 factor:1 | -1 (1.30628) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.07315 HOMO: -6.75659 LUMO: -0.03537 factor:1 | -1 (1.50084) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.21280 HOMO: -7.78518 LUMO: -2.36467 factor:1 | -1 (1.36120) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.16540 HOMO: -7.96477 LUMO: -2.75651 factor:1 | -1 (1.40860) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.16807 HOMO: -7.60286 LUMO: -2.35106 factor:1 | -1 (1.40593) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.87361 HOMO: -7.38245 LUMO: -1.21635 factor:1 | -1 (1.70039) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.62610 HOMO: -7.91579 LUMO: -1.50479 factor:1 | -1 (1.94790) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.86474 HOMO: -8.07362 LUMO: -0.28028 factor:1 | -1 (1.70926) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.58125 HOMO: -7.38245 LUMO: -1.15921 factor:1 | -1 (1.99274) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.62650 HOMO: -7.18653 LUMO: -0.94968 factor:1 | -1 (0.94750) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.14547 HOMO: -6.88448 LUMO: 0.38096 factor:1 | -1 (0.42852) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.60939 HOMO: -6.97972 LUMO: 0.43266 factor:1 | -1 (1.96461) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.32718 HOMO: -6.88992 LUMO: -0.43538 factor:1 | 1 (-0.75318) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19045 HOMO: -7.97021 LUMO: -0.17143 factor:1 | 1 (-0.61645) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84832 HOMO: -6.92530 LUMO: 0.77280 factor:1 | 1 (-0.27432) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.18027 HOMO: -7.89674 LUMO: -0.09796 factor:1 | 1 (-0.60627) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54962 HOMO: -7.02870 LUMO: 0.88709 factor:1 | -1 (0.02438) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.21552 HOMO: -6.78380 LUMO: 0.22041 factor:1 | -1 (0.35848) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24468 HOMO: -7.24911 LUMO: -0.82178 factor:1 | 1 (-0.67068) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65471 HOMO: -6.77019 LUMO: 0.52790 factor:1 | 1 (-0.08071) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29962 HOMO: -8.56070 LUMO: -1.83405 factor:1 | 1 (-0.72562) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82679 HOMO: -7.74164 LUMO: -2.36195 factor:1 | 1 (-0.25279) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77783 HOMO: -7.39878 LUMO: -2.41637 factor:1 | 1 (-1.20383) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.18846 HOMO: -7.61647 LUMO: -2.34018 factor:1 | 1 (-0.61446) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86951 HOMO: -6.93346 LUMO: -0.57688 factor:1 | 1 (-1.29551) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.71271 HOMO: -6.85183 LUMO: -1.00410 factor:1 | 1 (-1.13871) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83893 HOMO: -7.18925 LUMO: -1.12655 factor:1 | 1 (-0.26493) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92771 HOMO: -6.85183 LUMO: -1.60275 factor:1 | 1 (-1.35371) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.34588 HOMO: -7.51578 LUMO: 0.12517 factor:1 | 1 (-0.77188) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.32927 HOMO: -7.36068 LUMO: 0.05714 factor:1 | 1 (-1.75527) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48294 HOMO: -7.49674 LUMO: 0.18776 factor:1 | 1 (-0.90894) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.34856 HOMO: -7.09401 LUMO: -1.24900 factor:1 | 1 (-1.77456) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84485 HOMO: -7.22462 LUMO: -1.61364 factor:1 | 1 (-1.27085) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31502 HOMO: -7.74436 LUMO: -0.18776 factor:1 | 1 (-0.74102) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.03767 HOMO: -7.35252 LUMO: 0.75376 factor:1 | 1 (-1.46367) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62994 HOMO: -7.75252 LUMO: 0.00816 factor:1 | 1 (-1.05594) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15885 HOMO: -7.06680 LUMO: 0.24490 factor:1 | 1 (-0.58485) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01511 HOMO: -7.49129 LUMO: 0.14150 factor:1 | 1 (-1.44112) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94643 HOMO: -6.90625 LUMO: -1.11295 factor:1 | 1 (-1.37243) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24612 HOMO: -6.78380 LUMO: -0.93063 factor:1 | 1 (-0.67212) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89205 HOMO: -7.79878 LUMO: 0.30477 factor:1 | 1 (-0.31805) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21249 HOMO: -7.87498 LUMO: 0.61770 factor:1 | 1 (-0.63849) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.33655 HOMO: -7.23823 LUMO: 0.30205 factor:1 | -1 (0.23745) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89188 HOMO: -7.67633 LUMO: 0.13061 factor:1 | 1 (-0.31788) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45807 HOMO: -7.79606 LUMO: 0.34558 factor:1 | 1 (-0.88407) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70238 HOMO: -6.66135 LUMO: -2.60141 factor:1 | 1 (-0.12838) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.60658 HOMO: -7.03142 LUMO: 0.50885 factor:1 | -1 (0.96742) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73313 HOMO: -7.05591 LUMO: -0.06531 factor:1 | 1 (-0.15913) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.68228 HOMO: -7.45592 LUMO: -1.39594 factor:1 | -1 (0.89172) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83286 HOMO: -7.22462 LUMO: -1.10478 factor:1 | 1 (-0.25886) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.00773 HOMO: -8.14709 LUMO: -0.55783 factor:1 | -1 (0.56627) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.11470 HOMO: -7.22190 LUMO: -1.14560 factor:1 | -1 (3.45930) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.18147 HOMO: -7.28721 LUMO: -1.14016 factor:1 | -1 (3.39253) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11944.66293 HOMO: -6.97156 LUMO: 0.51702 factor:1 | -1 (3.91107) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26749 HOMO: -7.37156 LUMO: 0.29388 factor:1 | -1 (0.30651) | 1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45307 HOMO: -7.66273 LUMO: -1.59731 factor:1 | -1 (0.12093) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.17706 HOMO: -7.50490 LUMO: -1.49935 factor:1 | 1 (-0.60306) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.46799 HOMO: -7.61102 LUMO: -1.45581 factor:1 | -1 (1.10601) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95205 HOMO: -7.58653 LUMO: -1.61091 factor:1 | 1 (-0.37805) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85019 HOMO: -7.36068 LUMO: -1.14560 factor:1 | 1 (-0.27620) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19757 HOMO: -6.96339 LUMO: 0.26939 factor:1 | 1 (-0.62358) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14813 HOMO: -6.53617 LUMO: 0.22313 factor:1 | 1 (-0.57413) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.99155 HOMO: -7.33619 LUMO: -1.02587 factor:1 | -1 (1.58245) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.03313 HOMO: -6.87904 LUMO: 0.33742 factor:1 | -1 (1.54087) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.82847 HOMO: -6.88448 LUMO: 0.58777 factor:1 | -1 (1.74553) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51598 HOMO: -6.55522 LUMO: -1.51295 factor:1 | -1 (0.05801) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.62707 HOMO: -7.43415 LUMO: 0.10612 factor:1 | -1 (0.94693) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86130 HOMO: -7.54300 LUMO: -0.02449 factor:1 | 1 (-0.28730) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.92098 HOMO: -7.42054 LUMO: 0.28028 factor:1 | -1 (0.65302) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.97595 HOMO: -6.98244 LUMO: -0.95784 factor:1 | -1 (0.59805) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.83189 HOMO: -6.96884 LUMO: -1.12383 factor:1 | -1 (0.74211) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70548 HOMO: -6.80829 LUMO: -0.98233 factor:1 | 1 (-1.13148) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79614 HOMO: -7.60830 LUMO: 0.58504 factor:1 | 1 (-1.22214) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89193 HOMO: -7.52123 LUMO: 0.08163 factor:1 | 1 (-1.31793) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42966 HOMO: -7.59742 LUMO: 0.00272 factor:1 | 1 (-0.85566) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72466 HOMO: -6.99333 LUMO: -1.33880 factor:1 | 1 (-1.15066) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17433 HOMO: -6.63958 LUMO: -1.39322 factor:1 | 1 (-1.60033) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14122 HOMO: -7.86137 LUMO: 0.01633 factor:1 | 1 (-0.56722) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.10153 HOMO: -7.29537 LUMO: 0.14694 factor:1 | -1 (0.47247) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.06283 HOMO: -6.95523 LUMO: 0.48708 factor:1 | -1 (0.51117) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.12526 HOMO: -7.10217 LUMO: -1.10478 factor:1 | -1 (1.44873) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92655 HOMO: -6.88176 LUMO: -0.96328 factor:1 | 1 (-0.35255) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89649 HOMO: -7.89130 LUMO: -0.13334 factor:1 | -1 (0.67751) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73135 HOMO: -7.75252 LUMO: 0.25579 factor:1 | 1 (-1.15735) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41676 HOMO: -6.87632 LUMO: -0.93063 factor:1 | 1 (-0.84276) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.71274 HOMO: -6.78108 LUMO: -0.86804 factor:1 | 1 (-1.13874) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01174 HOMO: -5.98106 LUMO: 0.10340 factor:1 | 1 (-1.43774) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.07052 HOMO: -6.40284 LUMO: -0.87349 factor:1 | 1 (-1.49652) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50689 HOMO: -6.77019 LUMO: -1.20819 factor:1 | 1 (-0.93289) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.24987 HOMO: -6.90081 LUMO: -1.00682 factor:1 | 1 (-1.67587) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70651 HOMO: -6.59060 LUMO: -0.26667 factor:1 | 1 (-1.13251) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48074 HOMO: -6.50896 LUMO: -0.48708 factor:1 | 1 (-0.90674) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54000 HOMO: -6.20420 LUMO: -0.73471 factor:1 | 1 (-0.96600) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97746 HOMO: -6.17154 LUMO: -0.68573 factor:1 | 1 (-0.40346) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14356 HOMO: -6.21236 LUMO: 0.09796 factor:1 | 1 (-0.56956) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95939 HOMO: -6.38379 LUMO: 0.58232 factor:1 | 1 (-0.38539) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83938 HOMO: -7.42871 LUMO: 0.40273 factor:1 | 1 (-1.26538) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85209 HOMO: -6.54978 LUMO: 0.26395 factor:1 | 1 (-1.27809) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59762 HOMO: -7.14027 LUMO: 0.14150 factor:1 | 1 (-0.02362) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10459 HOMO: -7.25456 LUMO: -0.15783 factor:1 | 1 (-0.53059) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74486 HOMO: -6.90897 LUMO: 0.63403 factor:1 | 1 (-0.17086) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68213 HOMO: -6.49264 LUMO: 0.71022 factor:1 | 1 (-1.10813) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49932 HOMO: -6.56067 LUMO: -1.03947 factor:1 | 1 (-0.92532) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03191 HOMO: -6.79196 LUMO: -1.12655 factor:1 | 1 (-0.45791) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68308 HOMO: -6.95251 LUMO: -1.09118 factor:1 | 1 (-1.10908) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33586 HOMO: -7.47225 LUMO: -0.22041 factor:1 | 1 (-0.76186) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14046 HOMO: -7.13483 LUMO: -0.98505 factor:1 | 1 (-0.56646) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67520 HOMO: -6.99061 LUMO: -1.05852 factor:1 | 1 (-0.10120) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24609 HOMO: -6.52257 LUMO: -1.11022 factor:1 | 1 (-0.67209) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07006 HOMO: -6.75114 LUMO: -1.09934 factor:1 | 1 (-0.49606) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77226 HOMO: -6.82189 LUMO: -0.89253 factor:1 | 1 (-0.19826) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.90585 HOMO: -6.83278 LUMO: -0.97961 factor:1 | -1 (0.66815) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.92240 HOMO: -6.65318 LUMO: -0.84355 factor:1 | -1 (0.65160) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.59716 HOMO: -6.75931 LUMO: -0.88437 factor:1 | -1 (0.97683) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45898 HOMO: -6.19059 LUMO: -0.45715 factor:1 | -1 (0.11502) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61661 HOMO: -7.09673 LUMO: -2.01908 factor:1 | 1 (-0.04261) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84062 HOMO: -7.88042 LUMO: 0.38640 factor:1 | 1 (-0.26662) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.58880 HOMO: -7.83144 LUMO: 0.14422 factor:1 | 1 (-0.01480) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.78958 HOMO: -7.46408 LUMO: 0.44627 factor:1 | -1 (0.78442) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.79328 HOMO: -7.12394 LUMO: -2.04902 factor:1 | -1 (0.78072) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.44201 HOMO: -6.78380 LUMO: -1.11295 factor:1 | -1 (1.13199) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.32939 HOMO: -7.12938 LUMO: -0.23674 factor:1 | 1 (-0.75539) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57494 HOMO: -6.14705 LUMO: -0.20409 factor:1 | 1 (-1.00094) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72785 HOMO: -6.50080 LUMO: -0.28300 factor:1 | 1 (-0.15385) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74978 HOMO: -6.50352 LUMO: -0.62042 factor:1 | 1 (-1.17578) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68801 HOMO: -6.46543 LUMO: -0.53879 factor:1 | 1 (-1.11401) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51451 HOMO: -7.32803 LUMO: -0.52790 factor:1 | 1 (-0.94051) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.88757 HOMO: -5.94025 LUMO: -0.17687 factor:1 | 1 (-1.31358) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02114 HOMO: -5.62187 LUMO: 0.05714 factor:1 | 1 (-0.44714) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79702 HOMO: -7.03414 LUMO: -1.04492 factor:1 | 1 (-0.22302) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15809 HOMO: -6.75387 LUMO: -2.02181 factor:1 | 1 (-0.58409) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82078 HOMO: -6.55250 LUMO: -0.75648 factor:1 | 1 (-0.24678) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.46162 HOMO: -6.81101 LUMO: -1.02043 factor:1 | -1 (1.11237) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.66011 HOMO: -6.69672 LUMO: -2.81910 factor:1 | -1 (1.91389) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.99105 HOMO: -6.69128 LUMO: -2.58236 factor:1 | -1 (0.58295) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.07283 HOMO: -6.73482 LUMO: -2.06807 factor:1 | -1 (1.50117) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.36987 HOMO: -7.66545 LUMO: 0.17143 factor:1 | -1 (1.20413) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.64582 HOMO: -6.87904 LUMO: -1.25172 factor:1 | -1 (0.92818) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.73940 HOMO: -6.84366 LUMO: -0.19320 factor:1 | -1 (0.83460) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.45066 HOMO: -6.97972 LUMO: -0.97961 factor:1 | -1 (1.12334) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.85347 HOMO: -6.72121 LUMO: -0.70477 factor:1 | -1 (0.72053) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.89729 HOMO: -7.18925 LUMO: 0.40001 factor:1 | -1 (1.67671) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.96104 HOMO: -6.72121 LUMO: 0.19592 factor:1 | -1 (1.61295) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.65766 HOMO: -6.85999 LUMO: -0.39457 factor:1 | -1 (1.91633) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02606 HOMO: -6.90625 LUMO: 0.05987 factor:1 | 1 (-0.45206) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94869 HOMO: -7.00421 LUMO: 0.37552 factor:1 | 1 (-1.37469) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69802 HOMO: -6.56883 LUMO: -0.97689 factor:1 | 1 (-1.12402) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91142 HOMO: -6.66679 LUMO: 0.56055 factor:1 | 1 (-0.33742) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91161 HOMO: -6.75931 LUMO: 0.32926 factor:1 | 1 (-0.33761) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85128 HOMO: -6.53617 LUMO: -1.06397 factor:1 | 1 (-0.27728) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92496 HOMO: -6.78108 LUMO: 0.42722 factor:1 | 1 (-1.35096) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93402 HOMO: -7.05319 LUMO: 0.61498 factor:1 | 1 (-1.36003) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20756 HOMO: -6.78380 LUMO: 1.49391 factor:1 | 1 (-0.63356) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38686 HOMO: -7.21102 LUMO: 0.27211 factor:1 | 1 (-0.81286) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60815 HOMO: -6.67223 LUMO: 0.81362 factor:1 | 1 (-0.03415) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97119 HOMO: -6.69944 LUMO: 1.40683 factor:1 | 1 (-1.39720) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.27336 HOMO: -7.02598 LUMO: 1.46941 factor:1 | 1 (-0.69936) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99289 HOMO: -5.85045 LUMO: -0.76736 factor:1 | 1 (-0.41889) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90633 HOMO: -6.53890 LUMO: -0.50885 factor:1 | 1 (-0.33233) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.95791 HOMO: -6.42733 LUMO: -0.63947 factor:1 | -1 (0.61609) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.02365 HOMO: -6.82189 LUMO: -0.85444 factor:1 | -1 (0.55035) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.54353 HOMO: -6.97428 LUMO: -1.22179 factor:1 | -1 (1.03047) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.79880 HOMO: -6.93346 LUMO: -1.09934 factor:1 | -1 (0.77520) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00299 HOMO: -7.17292 LUMO: -1.11839 factor:1 | 1 (-0.42899) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04908 HOMO: -7.00965 LUMO: -1.23268 factor:1 | 1 (-0.47508) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72238 HOMO: -6.73210 LUMO: -1.12383 factor:1 | 1 (-0.14838) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.32865 HOMO: -7.61375 LUMO: -0.11973 factor:1 | 1 (-0.75465) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20563 HOMO: -7.42327 LUMO: 0.41906 factor:1 | 1 (-0.63163) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70698 HOMO: -6.94162 LUMO: -1.01771 factor:1 | 1 (-0.13298) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80962 HOMO: -6.82189 LUMO: -0.92791 factor:1 | 1 (-0.23562) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53353 HOMO: -6.92258 LUMO: -1.73881 factor:1 | 1 (-0.95953) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70809 HOMO: -6.50896 LUMO: -1.60819 factor:1 | 1 (-1.13409) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61342 HOMO: -6.38379 LUMO: -2.18780 factor:1 | 1 (-1.03942) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74557 HOMO: -6.48992 LUMO: -0.97417 factor:1 | 1 (-0.17157) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.56232 HOMO: -6.01644 LUMO: -0.04354 factor:1 | 1 (-0.98832) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93207 HOMO: -6.70761 LUMO: -0.14422 factor:1 | 1 (-0.35807) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77553 HOMO: -6.70216 LUMO: 0.14422 factor:1 | 1 (-0.20153) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.37361 HOMO: -7.07224 LUMO: -0.10885 factor:1 | 1 (-0.79961) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.64729 HOMO: -7.52667 LUMO: -0.74287 factor:1 | 1 (-2.07329) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.77877 HOMO: -6.48447 LUMO: -0.96056 factor:1 | 1 (-2.20478) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.24573 HOMO: -6.22597 LUMO: -0.41361 factor:1 | 1 (-1.67173) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26300 HOMO: -6.12256 LUMO: -1.05852 factor:1 | -1 (0.31100) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.32938 HOMO: -6.97428 LUMO: -0.60681 factor:1 | 1 (-1.75538) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.20089 HOMO: -6.78380 LUMO: -0.88981 factor:1 | 1 (-1.62689) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95428 HOMO: -6.85999 LUMO: 0.07891 factor:1 | 1 (-0.38028) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81574 HOMO: -7.08312 LUMO: -0.60137 factor:1 | 1 (-1.24174) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.38854 HOMO: -6.57699 LUMO: -0.68028 factor:1 | 1 (-1.81454) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.07147 HOMO: -6.09807 LUMO: -0.31837 factor:1 | 1 (-1.49747) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.09566 HOMO: -6.10624 LUMO: 0.14966 factor:1 | 1 (-1.52166) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19775 HOMO: -6.77019 LUMO: -0.95784 factor:1 | -1 (0.37625) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.12890 HOMO: -5.93208 LUMO: -0.44627 factor:1 | -1 (0.44510) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53892 HOMO: -6.12256 LUMO: -0.27756 factor:1 | -1 (0.03508) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74698 HOMO: -5.98106 LUMO: -0.37824 factor:1 | 1 (-0.17298) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.27243 HOMO: -7.06408 LUMO: -1.12927 factor:1 | 1 (-0.69843) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49222 HOMO: -6.70761 LUMO: -0.98505 factor:1 | 1 (-0.91822) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.14508 HOMO: -7.00965 LUMO: -0.42722 factor:1 | 1 (-1.57108) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98162 HOMO: -5.96201 LUMO: -0.59049 factor:1 | 1 (-1.40762) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.34230 HOMO: -6.34570 LUMO: -1.68438 factor:1 | 1 (-1.76830) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.11299 HOMO: -6.97156 LUMO: -1.85854 factor:1 | 1 (-1.53899) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85661 HOMO: -5.91848 LUMO: -2.51433 factor:1 | 1 (-1.28261) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.07672 HOMO: -6.39195 LUMO: -1.66262 factor:1 | 1 (-1.50272) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90036 HOMO: -6.50352 LUMO: 0.19592 factor:1 | 1 (-1.32636) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84459 HOMO: -6.45998 LUMO: 0.34831 factor:1 | 1 (-0.27059) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08978 HOMO: -7.05319 LUMO: 0.23402 factor:1 | 1 (-1.51578) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99019 HOMO: -6.61237 LUMO: 0.18232 factor:1 | 1 (-1.41619) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.24736 HOMO: -6.57427 LUMO: 0.40545 factor:1 | 1 (-1.67336) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23569 HOMO: -7.26544 LUMO: 0.41089 factor:1 | 1 (-1.66169) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76758 HOMO: -6.26406 LUMO: -0.85444 factor:1 | 1 (-0.19358) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77285 HOMO: -6.25318 LUMO: -0.79457 factor:1 | 1 (-1.19885) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94782 HOMO: -6.68040 LUMO: 0.41089 factor:1 | 1 (-1.37382) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09621 HOMO: -6.37835 LUMO: 0.37280 factor:1 | 1 (-0.52221) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91365 HOMO: -6.56067 LUMO: 0.62858 factor:1 | 1 (-0.33965) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71607 HOMO: -6.74026 LUMO: -0.04082 factor:1 | 1 (-0.14207) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90217 HOMO: -6.53617 LUMO: 0.35103 factor:1 | 1 (-0.32817) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76716 HOMO: -6.51985 LUMO: 0.25851 factor:1 | 1 (-1.19316) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.53327 HOMO: -6.58788 LUMO: -1.98371 factor:1 | 1 (-1.95927) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17542 HOMO: -6.51441 LUMO: 0.29116 factor:1 | 1 (-1.60142) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.16546 HOMO: -6.81101 LUMO: 0.35647 factor:1 | 1 (-1.59146) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79259 HOMO: -6.42733 LUMO: 0.10340 factor:1 | 1 (-0.21859) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81243 HOMO: -6.70761 LUMO: 0.28028 factor:1 | 1 (-0.23843) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54689 HOMO: -6.67495 LUMO: 0.01633 factor:1 | 1 (-0.97289) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68259 HOMO: -6.75387 LUMO: 0.15510 factor:1 | 1 (-1.10859) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52243 HOMO: -6.56067 LUMO: 0.35919 factor:1 | -1 (0.05157) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.42001 HOMO: -7.16748 LUMO: 0.21497 factor:1 | -1 (0.15399) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.40991 HOMO: -6.71849 LUMO: 0.26667 factor:1 | 1 (-0.83591) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55870 HOMO: -6.69128 LUMO: 0.55783 factor:1 | 1 (-0.98470) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91288 HOMO: -6.71305 LUMO: 0.45987 factor:1 | 1 (-1.33888) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45788 HOMO: -5.90487 LUMO: -0.70750 factor:1 | 1 (-0.88388) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.09947 HOMO: -6.84638 LUMO: -0.72110 factor:1 | 1 (-1.52547) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29981 HOMO: -6.66135 LUMO: -1.13471 factor:1 | 1 (-0.72581) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.58962 HOMO: -6.74026 LUMO: -0.64763 factor:1 | 1 (-0.01562) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78613 HOMO: -6.69672 LUMO: -1.05036 factor:1 | 1 (-1.21213) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01721 HOMO: -6.78924 LUMO: -1.03675 factor:1 | 1 (-1.44321) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.73230 HOMO: -6.81373 LUMO: -0.85988 factor:1 | 1 (-2.15830) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.67126 HOMO: -7.26544 LUMO: 0.91158 factor:1 | 1 (-2.09726) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89389 HOMO: -6.64230 LUMO: -1.92929 factor:1 | 1 (-1.31989) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57549 HOMO: -7.20830 LUMO: 0.11429 factor:1 | 1 (-1.00149) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.40908 HOMO: -7.17020 LUMO: 0.04898 factor:1 | 1 (-1.83508) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60047 HOMO: -7.16476 LUMO: 0.04898 factor:1 | 1 (-1.02647) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69394 HOMO: -6.59332 LUMO: -0.49253 factor:1 | 1 (-1.11994) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97341 HOMO: -7.46953 LUMO: 0.84083 factor:1 | 1 (-0.39941) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48928 HOMO: -7.39878 LUMO: 0.88709 factor:1 | 1 (-0.91528) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76184 HOMO: -6.84094 LUMO: -0.61498 factor:1 | 1 (-0.18784) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74094 HOMO: -6.03549 LUMO: -0.27211 factor:1 | 1 (-0.16694) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99681 HOMO: -7.31170 LUMO: -0.64763 factor:1 | 1 (-0.42281) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87791 HOMO: -6.88992 LUMO: -0.84627 factor:1 | 1 (-1.30392) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12394 HOMO: -7.12666 LUMO: -0.09252 factor:1 | 1 (-0.54994) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.00076 HOMO: -6.70489 LUMO: -0.63675 factor:1 | 1 (-2.42677) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.62005 HOMO: -6.98788 LUMO: 0.86804 factor:1 | 1 (-2.04605) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90662 HOMO: -6.80285 LUMO: -0.60954 factor:1 | 1 (-1.33262) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62897 HOMO: -7.02054 LUMO: -0.74287 factor:1 | 1 (-0.05497) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80224 HOMO: -7.03686 LUMO: -0.81090 factor:1 | 1 (-1.22824) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88211 HOMO: -6.70489 LUMO: -1.00954 factor:1 | 1 (-0.30811) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14810 HOMO: -7.69810 LUMO: 0.00544 factor:1 | 1 (-0.57411) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.32980 HOMO: -6.83550 LUMO: -0.11157 factor:1 | 1 (-0.75580) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38460 HOMO: -6.76203 LUMO: -2.13609 factor:1 | 1 (-0.81060) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87175 HOMO: -6.72121 LUMO: -2.62862 factor:1 | 1 (-0.29775) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85354 HOMO: -6.48719 LUMO: -2.73474 factor:1 | 1 (-0.27954) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00201 HOMO: -6.83006 LUMO: -0.00544 factor:1 | 1 (-0.42801) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12457 HOMO: -6.84094 LUMO: -1.11022 factor:1 | 1 (-0.55057) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15031 HOMO: -6.66951 LUMO: -1.23812 factor:1 | 1 (-0.57631) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77277 HOMO: -6.78380 LUMO: -1.27894 factor:1 | 1 (-1.19877) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91493 HOMO: -6.50352 LUMO: -0.56055 factor:1 | 1 (-0.34093) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70626 HOMO: -7.77974 LUMO: -0.26395 factor:1 | 1 (-1.13227) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.42056 HOMO: -7.01510 LUMO: -1.64085 factor:1 | 1 (-1.84656) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.57458 HOMO: -6.59876 LUMO: -0.91158 factor:1 | 1 (-2.00058) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97492 HOMO: -4.67219 LUMO: -0.67756 factor:1 | 1 (-1.40092) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.29825 HOMO: -6.70489 LUMO: -0.65579 factor:1 | 1 (-1.72425) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.21387 HOMO: -6.62325 LUMO: -0.60409 factor:1 | 1 (-1.63987) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.02311 HOMO: -6.20147 LUMO: 0.15238 factor:1 | 1 (-1.44912) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.26522 HOMO: -6.43549 LUMO: -0.07075 factor:1 | 1 (-0.69122) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.78544 HOMO: -7.02054 LUMO: 0.13061 factor:1 | 1 (-2.21144) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.66361 HOMO: -7.04503 LUMO: 0.30749 factor:1 | 1 (-3.08961) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.77807 HOMO: -6.74842 LUMO: -0.99594 factor:1 | 1 (-2.20407) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.95714 HOMO: -6.35658 LUMO: 0.41633 factor:1 | 1 (-2.38315) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17879 HOMO: -6.79740 LUMO: 0.56872 factor:1 | 1 (-1.60479) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.13256 HOMO: -6.51713 LUMO: -0.05987 factor:1 | 1 (-1.55856) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.80403 HOMO: -6.68040 LUMO: 0.34558 factor:1 | 1 (-2.23003) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.22538 HOMO: -6.39740 LUMO: 0.50069 factor:1 | 1 (-1.65138) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.40998 HOMO: -6.91713 LUMO: -0.97145 factor:1 | 1 (-1.83598) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99351 HOMO: -7.10761 LUMO: -0.27483 factor:1 | 1 (-1.41951) | 1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.18510 HOMO: -6.98788 LUMO: 0.40273 factor:1 | 1 (-1.61110) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01941 HOMO: -6.87087 LUMO: 0.28572 factor:1 | 1 (-1.44541) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93020 HOMO: -7.36612 LUMO: -0.12245 factor:1 | 1 (-0.35620) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17705 HOMO: -6.72938 LUMO: 0.33742 factor:1 | 1 (-1.60305) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48782 HOMO: -7.32531 LUMO: 0.07619 factor:1 | -1 (0.08618) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23329 HOMO: -6.87087 LUMO: -0.08436 factor:1 | 1 (-1.65930) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.28480 HOMO: -6.67495 LUMO: 0.85988 factor:1 | -1 (0.28920) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.33022 HOMO: -6.96339 LUMO: 0.65307 factor:1 | 1 (-1.75622) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.22459 HOMO: -6.58516 LUMO: -0.78641 factor:1 | 1 (-1.65059) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93123 HOMO: -6.56883 LUMO: 0.44355 factor:1 | 1 (-0.35723) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36969 HOMO: -6.68312 LUMO: 0.43538 factor:1 | 1 (-0.79569) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42060 HOMO: -6.81917 LUMO: 0.20681 factor:1 | 1 (-0.84660) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.56800 HOMO: -6.91169 LUMO: 0.08163 factor:1 | 1 (-0.99400) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67299 HOMO: -4.88444 LUMO: -0.49253 factor:1 | 1 (-1.09899) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52036 HOMO: -6.42189 LUMO: 0.64763 factor:1 | 1 (-0.94636) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52974 HOMO: -6.24501 LUMO: 0.55783 factor:1 | 1 (-0.95575) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69326 HOMO: -6.41372 LUMO: 0.29388 factor:1 | 1 (-1.11926) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70020 HOMO: -5.67902 LUMO: 1.77690 factor:1 | 1 (-1.12620) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.58719 HOMO: -6.55794 LUMO: 0.05170 factor:1 | 1 (-1.01319) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98651 HOMO: -6.52801 LUMO: 0.25851 factor:1 | 1 (-1.41252) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81024 HOMO: -7.08857 LUMO: 0.11157 factor:1 | 1 (-1.23624) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06401 HOMO: -6.58243 LUMO: 0.75648 factor:1 | 1 (-1.49001) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.31901 HOMO: -7.22190 LUMO: 0.45171 factor:1 | 1 (-1.74501) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.03794 HOMO: -6.47087 LUMO: 0.00000 factor:1 | 1 (-1.46395) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.43322 HOMO: -6.78652 LUMO: 1.32247 factor:1 | 1 (-1.85922) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51785 HOMO: -6.74026 LUMO: 1.45309 factor:1 | 1 (-0.94385) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65633 HOMO: -6.69944 LUMO: 0.76464 factor:1 | 1 (-1.08233) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78480 HOMO: -6.62325 LUMO: 0.64763 factor:1 | 1 (-1.21080) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99334 HOMO: -6.45182 LUMO: 0.49253 factor:1 | 1 (-1.41935) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77941 HOMO: -7.14843 LUMO: 0.62586 factor:1 | 1 (-1.20541) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.00177 HOMO: -6.87087 LUMO: 1.53200 factor:1 | 1 (-2.42777) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81253 HOMO: -6.54978 LUMO: 0.45171 factor:1 | 1 (-0.23854) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70701 HOMO: -6.63686 LUMO: 0.80001 factor:1 | 1 (-0.13301) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.69864 HOMO: -7.00693 LUMO: 1.56193 factor:1 | 1 (-2.12464) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06418 HOMO: -6.02460 LUMO: 1.72792 factor:1 | 1 (-1.49018) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70836 HOMO: -6.36746 LUMO: -1.20002 factor:1 | 1 (-1.13436) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69323 HOMO: -7.26816 LUMO: -1.06397 factor:1 | 1 (-1.11923) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53826 HOMO: -7.34707 LUMO: -1.09662 factor:1 | 1 (-0.96426) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28808 HOMO: -7.93212 LUMO: -0.13606 factor:1 | 1 (-0.71408) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28560 HOMO: -6.80285 LUMO: 0.58504 factor:1 | 1 (-0.71160) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68526 HOMO: -7.12938 LUMO: 0.32926 factor:1 | 1 (-1.11126) | 1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42117 HOMO: -6.86815 LUMO: -1.30070 factor:1 | 1 (-0.84717) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.46889 HOMO: -6.99333 LUMO: -1.03947 factor:1 | 1 (-1.89489) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01313 HOMO: -7.56749 LUMO: -0.11157 factor:1 | 1 (-1.43913) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98009 HOMO: -7.57293 LUMO: -0.07891 factor:1 | 1 (-1.40609) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.13825 HOMO: -7.30626 LUMO: 0.27211 factor:1 | 1 (-1.56425) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93343 HOMO: -7.77974 LUMO: 0.27211 factor:1 | 1 (-0.35944) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99950 HOMO: -7.11578 LUMO: 0.19864 factor:1 | 1 (-0.42550) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.17064 HOMO: -7.71171 LUMO: 0.57688 factor:1 | 1 (-0.59664) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90840 HOMO: -7.83688 LUMO: 0.37824 factor:1 | 1 (-0.33440) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65073 HOMO: -6.94979 LUMO: -1.66534 factor:1 | 1 (-0.07674) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.05074 HOMO: -6.97156 LUMO: -1.13199 factor:1 | -1 (2.52326) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.23597 HOMO: -6.91441 LUMO: -1.08301 factor:1 | -1 (2.33803) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62181 HOMO: -6.71849 LUMO: -0.74831 factor:1 | 1 (-0.04781) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21053 HOMO: -7.09401 LUMO: -1.77690 factor:1 | 1 (-0.63653) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76151 HOMO: -6.97156 LUMO: -1.45037 factor:1 | 1 (-0.18751) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31951 HOMO: -7.22462 LUMO: -1.11295 factor:1 | 1 (-0.74551) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26763 HOMO: -7.85321 LUMO: 0.16599 factor:1 | -1 (0.30637) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.98825 HOMO: -7.71987 LUMO: 0.55511 factor:1 | -1 (0.58575) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.39846 HOMO: -7.63551 LUMO: 0.14422 factor:1 | -1 (0.17554) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.00558 HOMO: -6.98788 LUMO: -0.80546 factor:1 | -1 (0.56842) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.94219 HOMO: -6.98788 LUMO: -1.16737 factor:1 | -1 (1.63181) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.84869 HOMO: -6.56611 LUMO: -1.60819 factor:1 | -1 (1.72531) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95439 HOMO: -6.95251 LUMO: 0.66396 factor:1 | 1 (-0.38039) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07736 HOMO: -7.35252 LUMO: 0.49797 factor:1 | 1 (-0.50336) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09853 HOMO: -6.90897 LUMO: -0.81090 factor:1 | 1 (-0.52453) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07722 HOMO: -7.04503 LUMO: -1.08301 factor:1 | 1 (-0.50322) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.42975 HOMO: -6.92530 LUMO: -1.29526 factor:1 | -1 (0.14425) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08770 HOMO: -6.93074 LUMO: -1.25444 factor:1 | 1 (-0.51370) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43405 HOMO: -6.73482 LUMO: -0.62042 factor:1 | -1 (0.13995) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29837 HOMO: -7.67633 LUMO: 0.59593 factor:1 | -1 (0.27562) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87958 HOMO: -7.39061 LUMO: -0.19320 factor:1 | 1 (-0.30558) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.18100 HOMO: -7.55388 LUMO: -0.20136 factor:1 | 1 (-0.60700) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55887 HOMO: -7.14027 LUMO: -0.99866 factor:1 | -1 (0.01513) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.27179 HOMO: -6.75931 LUMO: -0.73199 factor:1 | -1 (0.30221) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45321 HOMO: -5.45044 LUMO: -0.18776 factor:1 | -1 (0.12079) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90913 HOMO: -6.70761 LUMO: -0.84083 factor:1 | 1 (-0.33514) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02492 HOMO: -6.05453 LUMO: -1.06669 factor:1 | 1 (-0.45092) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.22210 HOMO: -6.86815 LUMO: -0.98233 factor:1 | -1 (0.35190) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22430 HOMO: -6.73210 LUMO: -0.95240 factor:1 | 1 (-0.65030) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73851 HOMO: -5.89671 LUMO: -1.05036 factor:1 | 1 (-1.16451) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65966 HOMO: -7.61102 LUMO: 0.33470 factor:1 | 1 (-0.08566) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44572 HOMO: -7.51034 LUMO: 0.23674 factor:1 | -1 (0.12827) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57999 HOMO: -7.41510 LUMO: 0.62858 factor:1 | 1 (-0.00599) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84380 HOMO: -6.76203 LUMO: -1.72792 factor:1 | 1 (-0.26980) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79166 HOMO: -6.60420 LUMO: -0.45715 factor:1 | 1 (-0.21766) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89384 HOMO: -6.59060 LUMO: -0.58232 factor:1 | 1 (-0.31984) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78524 HOMO: -7.43687 LUMO: -0.76736 factor:1 | 1 (-0.21124) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75645 HOMO: -6.08719 LUMO: -0.48708 factor:1 | 1 (-0.18245) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68444 HOMO: -5.88854 LUMO: -0.05714 factor:1 | 1 (-1.11044) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97161 HOMO: -7.34435 LUMO: -0.71838 factor:1 | 1 (-0.39761) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05961 HOMO: -7.46408 LUMO: -0.63130 factor:1 | 1 (-0.48561) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.71773 HOMO: -7.00965 LUMO: -1.24900 factor:1 | -1 (2.85627) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44011 HOMO: -6.91169 LUMO: -0.88981 factor:1 | 1 (-0.86611) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01246 HOMO: -6.78652 LUMO: -0.82178 factor:1 | 1 (-0.43846) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15322 HOMO: -7.80423 LUMO: 0.87076 factor:1 | 1 (-0.57922) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.41552 HOMO: -6.97700 LUMO: -1.00954 factor:1 | -1 (0.15848) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87054 HOMO: -6.92530 LUMO: -0.88165 factor:1 | 1 (-1.29654) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73195 HOMO: -7.14571 LUMO: -1.04492 factor:1 | 1 (-1.15795) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13259 HOMO: -7.49674 LUMO: 0.34558 factor:1 | 1 (-0.55860) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85166 HOMO: -6.44094 LUMO: -1.20819 factor:1 | 1 (-1.27766) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24566 HOMO: -6.47359 LUMO: -1.14016 factor:1 | 1 (-0.67166) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82850 HOMO: -6.61237 LUMO: -0.87076 factor:1 | 1 (-1.25450) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36574 HOMO: -6.73754 LUMO: -1.09662 factor:1 | 1 (-0.79174) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65584 HOMO: -6.97700 LUMO: 0.13061 factor:1 | 1 (-1.08184) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.02206 HOMO: -6.82734 LUMO: 0.59865 factor:1 | -1 (2.55194) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.86363 HOMO: -6.86543 LUMO: -0.91430 factor:1 | -1 (1.71037) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.29585 HOMO: -6.74298 LUMO: 0.28028 factor:1 | -1 (1.27815) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.45945 HOMO: -6.75387 LUMO: 0.19592 factor:1 | -1 (1.11455) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72817 HOMO: -7.05591 LUMO: 0.10612 factor:1 | 1 (-1.15417) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80485 HOMO: -6.86543 LUMO: 0.49253 factor:1 | 1 (-1.23085) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89685 HOMO: -6.11440 LUMO: -1.12655 factor:1 | 1 (-1.32285) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29181 HOMO: -6.77291 LUMO: -1.02859 factor:1 | 1 (-0.71781) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59658 HOMO: -6.54978 LUMO: 0.29116 factor:1 | 1 (-1.02258) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86926 HOMO: -7.18108 LUMO: 0.00000 factor:1 | 1 (-1.29526) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.26677 HOMO: -6.86271 LUMO: -1.15376 factor:1 | 1 (-0.69277) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74938 HOMO: -6.78108 LUMO: -1.22723 factor:1 | 1 (-0.17538) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82549 HOMO: -6.40828 LUMO: 0.02449 factor:1 | 1 (-0.25149) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01319 HOMO: -6.43821 LUMO: 0.09796 factor:1 | 1 (-0.43919) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55732 HOMO: -6.99877 LUMO: 0.40545 factor:1 | -1 (0.01668) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63359 HOMO: -6.68856 LUMO: 0.19320 factor:1 | 1 (-0.05959) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69637 HOMO: -7.11034 LUMO: 0.31293 factor:1 | 1 (-0.12237) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87632 HOMO: -6.92530 LUMO: -0.85444 factor:1 | 1 (-0.30232) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02293 HOMO: -6.60148 LUMO: -0.59865 factor:1 | 1 (-0.44893) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84326 HOMO: -6.72938 LUMO: 0.30749 factor:1 | 1 (-0.26926) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47353 HOMO: -7.31170 LUMO: 0.06803 factor:1 | 1 (-0.89953) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.34043 HOMO: -7.09129 LUMO: -0.04626 factor:1 | 1 (-0.76644) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03357 HOMO: -6.38379 LUMO: -0.76736 factor:1 | 1 (-0.45957) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72045 HOMO: -6.13617 LUMO: -0.63947 factor:1 | 1 (-0.14645) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83988 HOMO: -6.92258 LUMO: 0.37007 factor:1 | 1 (-0.26588) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.29444 HOMO: -6.35930 LUMO: 0.41361 factor:1 | -1 (1.27956) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87884 HOMO: -6.60420 LUMO: 0.26667 factor:1 | 1 (-1.30484) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72235 HOMO: -6.04909 LUMO: 1.82588 factor:1 | 1 (-1.14835) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64229 HOMO: -6.69672 LUMO: 1.72520 factor:1 | 1 (-1.06829) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53438 HOMO: -6.50080 LUMO: 0.29116 factor:1 | -1 (0.03962) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.19955 HOMO: -6.60692 LUMO: -0.43266 factor:1 | 1 (-1.62555) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90621 HOMO: -6.93890 LUMO: 0.39729 factor:1 | 1 (-1.33222) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86232 HOMO: -6.52801 LUMO: -0.47076 factor:1 | 1 (-1.28832) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82812 HOMO: -6.41100 LUMO: 0.30477 factor:1 | 1 (-1.25412) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55607 HOMO: -6.37291 LUMO: -0.80001 factor:1 | -1 (0.01793) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23104 HOMO: -6.51985 LUMO: 1.44765 factor:1 | 1 (-1.65704) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.46590 HOMO: -6.64774 LUMO: 0.04626 factor:1 | 1 (-1.89190) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.50339 HOMO: -6.65863 LUMO: 0.29933 factor:1 | 1 (-1.92940) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97517 HOMO: -7.09673 LUMO: 0.28300 factor:1 | 1 (-1.40117) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.19367 HOMO: -6.57155 LUMO: -1.11567 factor:1 | 1 (-1.61968) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80538 HOMO: -6.38379 LUMO: -0.60681 factor:1 | 1 (-0.23138) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66814 HOMO: -6.60148 LUMO: 0.18232 factor:1 | 1 (-1.09414) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47456 HOMO: -6.96067 LUMO: -0.52246 factor:1 | 1 (-0.90056) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08682 HOMO: -6.57427 LUMO: -0.84627 factor:1 | 1 (-0.51283) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88500 HOMO: -6.59332 LUMO: -0.98233 factor:1 | 1 (-0.31100) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63473 HOMO: -6.20692 LUMO: -0.27483 factor:1 | 1 (-1.06073) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.42970 HOMO: -6.81373 LUMO: 0.74559 factor:1 | -1 (0.14430) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17727 HOMO: -6.60420 LUMO: 0.54695 factor:1 | 1 (-1.60327) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65097 HOMO: -6.58788 LUMO: -0.31021 factor:1 | 1 (-1.07697) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00094 HOMO: -6.72938 LUMO: 0.64763 factor:1 | 1 (-1.42694) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.30772 HOMO: -6.86815 LUMO: 0.32109 factor:1 | 1 (-1.73372) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54551 HOMO: -6.63141 LUMO: 0.18776 factor:1 | -1 (0.02849) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.60187 HOMO: -7.18653 LUMO: 0.09524 factor:1 | 1 (-2.02787) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90001 HOMO: -6.83550 LUMO: 0.03537 factor:1 | 1 (-1.32601) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.75122 HOMO: -7.47769 LUMO: 0.40817 factor:1 | 1 (-1.17722) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80265 HOMO: -6.57971 LUMO: -0.63675 factor:1 | 1 (-1.22865) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.53784 HOMO: -6.74842 LUMO: -0.16327 factor:1 | 1 (-1.96385) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.37295 HOMO: -7.07224 LUMO: 0.61770 factor:1 | 1 (-0.79895) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97805 HOMO: -6.83006 LUMO: 0.54695 factor:1 | 1 (-1.40405) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98964 HOMO: -6.60148 LUMO: 1.23540 factor:1 | 1 (-1.41565) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20408 HOMO: -6.99061 LUMO: 0.41089 factor:1 | 1 (-0.63008) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.23262 HOMO: -6.63686 LUMO: 0.85172 factor:1 | 1 (-0.65862) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51927 HOMO: -6.50624 LUMO: 0.12517 factor:1 | 1 (-0.94527) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48536 HOMO: -6.35658 LUMO: 0.36463 factor:1 | 1 (-0.91136) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30046 HOMO: -6.34570 LUMO: 0.65035 factor:1 | 1 (-0.72646) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61209 HOMO: -6.63141 LUMO: 1.25717 factor:1 | 1 (-1.03809) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47040 HOMO: -6.91441 LUMO: 1.32792 factor:1 | 1 (-0.89640) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47587 HOMO: -7.15387 LUMO: 0.64219 factor:1 | 1 (-0.90187) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.82651 HOMO: -7.17836 LUMO: 0.60409 factor:1 | 1 (-1.25251) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38969 HOMO: -6.92258 LUMO: 0.49525 factor:1 | 1 (-0.81569) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49581 HOMO: -6.31032 LUMO: 0.48708 factor:1 | 1 (-0.92181) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41829 HOMO: -6.49808 LUMO: 0.31021 factor:1 | 1 (-0.84429) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42765 HOMO: -6.48447 LUMO: 0.37552 factor:1 | 1 (-0.85365) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52836 HOMO: -6.66135 LUMO: -1.08301 factor:1 | 1 (-0.95436) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67693 HOMO: -6.33481 LUMO: -0.51974 factor:1 | 1 (-1.10293) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52457 HOMO: -6.76475 LUMO: -0.15238 factor:1 | 1 (-0.95058) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51334 HOMO: -6.93346 LUMO: -0.10885 factor:1 | 1 (-0.93934) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42786 HOMO: -7.19741 LUMO: 0.73199 factor:1 | 1 (-0.85387) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99258 HOMO: -6.82734 LUMO: 0.88437 factor:1 | 1 (-1.41858) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13093 HOMO: -7.01237 LUMO: 0.02721 factor:1 | 1 (-0.55694) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39293 HOMO: -6.39195 LUMO: 1.46941 factor:1 | 1 (-0.81893) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29785 HOMO: -6.53890 LUMO: 1.32792 factor:1 | 1 (-0.72385) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53527 HOMO: -6.82734 LUMO: 1.98099 factor:1 | 1 (-0.96127) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42465 HOMO: -6.74570 LUMO: 1.68983 factor:1 | 1 (-0.85066) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55181 HOMO: -6.41100 LUMO: 1.39050 factor:1 | 1 (-0.97781) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45701 HOMO: -5.92664 LUMO: 1.65989 factor:1 | 1 (-0.88301) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63297 HOMO: -6.07630 LUMO: 1.54833 factor:1 | 1 (-0.05897) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44479 HOMO: -6.45998 LUMO: 0.68573 factor:1 | 1 (-0.87079) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.79594 HOMO: -6.52801 LUMO: 0.41361 factor:1 | 1 (-2.22195) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35761 HOMO: -6.77564 LUMO: 0.42178 factor:1 | 1 (-0.78361) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.20886 HOMO: -6.56339 LUMO: 1.65717 factor:1 | 1 (-1.63486) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.79442 HOMO: -5.85861 LUMO: 1.90752 factor:1 | 1 (-2.22042) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29636 HOMO: -6.77019 LUMO: -2.48440 factor:1 | -1 (0.27764) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.25907 HOMO: -6.53890 LUMO: -1.82588 factor:1 | 1 (-0.68507) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94239 HOMO: -6.50352 LUMO: -1.66806 factor:1 | 1 (-0.36839) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.04314 HOMO: -6.90625 LUMO: 0.43538 factor:1 | 1 (-1.46914) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43167 HOMO: -6.85455 LUMO: 0.53062 factor:1 | 1 (-0.85768) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.22289 HOMO: -6.49536 LUMO: 0.31021 factor:1 | -1 (0.35111) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12361 HOMO: -4.97696 LUMO: -0.09252 factor:1 | 1 (-0.54962) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22313 HOMO: -5.31166 LUMO: 0.34286 factor:1 | 1 (-0.64913) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.16332 HOMO: -6.42461 LUMO: 0.74287 factor:1 | -1 (0.41067) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.16311 HOMO: -6.59604 LUMO: 0.62858 factor:1 | -1 (0.41089) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.22357 HOMO: -6.45998 LUMO: -0.61770 factor:1 | -1 (0.35043) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.22548 HOMO: -6.75659 LUMO: -0.34014 factor:1 | -1 (0.34852) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.21157 HOMO: -6.63958 LUMO: 0.36191 factor:1 | -1 (0.36243) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.27655 HOMO: -5.92936 LUMO: -0.67484 factor:1 | -1 (0.29745) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.99992 HOMO: -5.67630 LUMO: 1.80956 factor:1 | -1 (0.57408) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05116 HOMO: -6.50352 LUMO: -0.78369 factor:1 | -1 (0.52284) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80973 HOMO: -6.35930 LUMO: -0.75648 factor:1 | 1 (-0.23573) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.16901 HOMO: -6.74298 LUMO: 0.48980 factor:1 | -1 (0.40499) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.34714 HOMO: -6.85183 LUMO: 0.15510 factor:1 | -1 (0.22686) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.98316 HOMO: -6.90897 LUMO: 0.26123 factor:1 | -1 (0.59084) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35054 HOMO: -6.85999 LUMO: 0.47892 factor:1 | -1 (0.22346) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75966 HOMO: -6.69944 LUMO: 0.57416 factor:1 | 1 (-0.18566) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43623 HOMO: -6.74026 LUMO: 0.69933 factor:1 | -1 (0.13777) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85678 HOMO: -6.52801 LUMO: 0.75376 factor:1 | 1 (-0.28278) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85956 HOMO: -7.05863 LUMO: 0.44627 factor:1 | 1 (-0.28556) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44156 HOMO: -6.96339 LUMO: 0.48164 factor:1 | -1 (0.13244) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.25742 HOMO: -6.95795 LUMO: 0.44355 factor:1 | -1 (0.31658) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49219 HOMO: -6.36746 LUMO: 0.58777 factor:1 | 1 (-0.91819) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55432 HOMO: -6.69400 LUMO: 0.40545 factor:1 | 1 (-0.98032) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21782 HOMO: -6.30760 LUMO: -0.66668 factor:1 | 1 (-0.64382) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95066 HOMO: -6.53617 LUMO: -0.64491 factor:1 | 1 (-0.37666) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98130 HOMO: -6.80829 LUMO: 0.17415 factor:1 | 1 (-0.40730) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99074 HOMO: -6.80285 LUMO: 0.73471 factor:1 | 1 (-0.41674) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06630 HOMO: -6.43821 LUMO: 0.21769 factor:1 | 1 (-1.49230) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91253 HOMO: -6.98788 LUMO: 0.10885 factor:1 | 1 (-1.33853) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.91860 HOMO: -7.15115 LUMO: 0.40817 factor:1 | 1 (-1.34460) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29314 HOMO: -6.00011 LUMO: -0.98505 factor:1 | 1 (-0.71914) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74474 HOMO: -6.16882 LUMO: -0.77825 factor:1 | 1 (-1.17074) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76213 HOMO: -6.30760 LUMO: 0.34831 factor:1 | 1 (-1.18813) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20808 HOMO: -6.64502 LUMO: 0.63403 factor:1 | 1 (-0.63408) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29277 HOMO: -6.93618 LUMO: 0.96600 factor:1 | -1 (0.28123) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.32863 HOMO: -6.45182 LUMO: 0.16327 factor:1 | -1 (0.24537) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.23089 HOMO: -6.99605 LUMO: 0.20953 factor:1 | -1 (0.34311) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.09350 HOMO: -6.72665 LUMO: 0.32654 factor:1 | -1 (0.48050) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50569 HOMO: -6.38379 LUMO: 0.45443 factor:1 | 1 (-0.93169) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.11707 HOMO: -6.65318 LUMO: 0.04354 factor:1 | -1 (0.45693) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11088 HOMO: -6.94707 LUMO: -1.68438 factor:1 | 1 (-0.53688) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00745 HOMO: -6.71849 LUMO: 0.15783 factor:1 | 1 (-0.43345) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93188 HOMO: -6.97156 LUMO: 0.43266 factor:1 | 1 (-0.35788) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85825 HOMO: -6.91441 LUMO: -0.54695 factor:1 | 1 (-0.28425) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86287 HOMO: -6.74842 LUMO: -0.76192 factor:1 | 1 (-0.28888) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02824 HOMO: -6.70489 LUMO: 0.19048 factor:1 | 1 (-0.45424) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03956 HOMO: -7.25728 LUMO: 0.33470 factor:1 | 1 (-0.46556) | 1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63000 HOMO: -6.96339 LUMO: 0.55511 factor:1 | 1 (-0.05600) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70649 HOMO: -6.77564 LUMO: 0.72382 factor:1 | 1 (-0.13249) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43587 HOMO: -6.75387 LUMO: 0.39729 factor:1 | -1 (0.13812) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69787 HOMO: -7.00149 LUMO: 0.06531 factor:1 | 1 (-0.12387) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84726 HOMO: -7.09945 LUMO: 0.33470 factor:1 | 1 (-0.27326) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.25687 HOMO: -7.20830 LUMO: 0.59593 factor:1 | 1 (-0.68287) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00216 HOMO: -6.40556 LUMO: 0.56600 factor:1 | 1 (-1.42816) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.60944 HOMO: -6.77291 LUMO: 0.73471 factor:1 | 1 (-2.03544) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83098 HOMO: -6.65046 LUMO: 0.09796 factor:1 | 1 (-0.25698) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87898 HOMO: -6.95795 LUMO: 0.22313 factor:1 | 1 (-0.30499) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84352 HOMO: -6.85727 LUMO: 0.04626 factor:1 | 1 (-1.26952) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73104 HOMO: -7.27360 LUMO: 0.42178 factor:1 | 1 (-0.15704) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71770 HOMO: -6.78924 LUMO: -0.13334 factor:1 | 1 (-0.14370) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.75027 HOMO: -6.63141 LUMO: 0.38368 factor:1 | 1 (-1.17627) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11303 HOMO: -6.92258 LUMO: 0.39184 factor:1 | 1 (-0.53903) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69911 HOMO: -6.19331 LUMO: -0.46804 factor:1 | 1 (-1.12511) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69991 HOMO: -7.26544 LUMO: -0.05442 factor:1 | 1 (-0.12591) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.32383 HOMO: -7.09401 LUMO: 0.30749 factor:1 | -1 (1.25017) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.74733 HOMO: -6.14705 LUMO: -0.88709 factor:1 | -1 (1.82667) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.29313 HOMO: -6.53617 LUMO: -0.28572 factor:1 | -1 (1.28087) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06424 HOMO: -6.37291 LUMO: -0.67212 factor:1 | 1 (-0.49024) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65952 HOMO: -6.65591 LUMO: 0.03810 factor:1 | 1 (-0.08553) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.55526 HOMO: -7.11034 LUMO: 0.75103 factor:1 | -1 (1.01874) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96446 HOMO: -6.85183 LUMO: -0.05987 factor:1 | 1 (-0.39046) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00378 HOMO: -6.70761 LUMO: -0.05442 factor:1 | 1 (-0.42978) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.66334 HOMO: -6.23413 LUMO: 0.06259 factor:1 | -1 (0.91066) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78908 HOMO: -6.55794 LUMO: 0.74015 factor:1 | 1 (-0.21508) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.17115 HOMO: -7.27905 LUMO: 0.26939 factor:1 | 1 (-0.59715) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.23390 HOMO: -6.34842 LUMO: -0.86804 factor:1 | 1 (-0.65990) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35067 HOMO: -6.27222 LUMO: 1.46125 factor:1 | 1 (-0.77667) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38822 HOMO: -6.65046 LUMO: 2.04902 factor:1 | 1 (-0.81422) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.96899 HOMO: -7.11850 LUMO: -1.14016 factor:1 | -1 (1.60501) | 1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87806 HOMO: -6.88720 LUMO: -1.20274 factor:1 | 1 (-0.30406) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.01165 HOMO: -6.69400 LUMO: -0.31565 factor:1 | -1 (0.56235) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.80824 HOMO: -6.95523 LUMO: -1.55377 factor:1 | -1 (0.76576) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.02858 HOMO: -6.41372 LUMO: -0.83539 factor:1 | -1 (1.54542) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.12437 HOMO: -6.13889 LUMO: -0.90070 factor:1 | -1 (1.44963) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.08945 HOMO: -6.44366 LUMO: -0.55511 factor:1 | -1 (1.48454) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.12148 HOMO: -6.10079 LUMO: -0.71022 factor:1 | -1 (1.45252) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06628 HOMO: -6.90353 LUMO: -0.64763 factor:1 | 1 (-0.49228) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.23421 HOMO: -6.65046 LUMO: -0.82450 factor:1 | -1 (0.33979) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57833 HOMO: -6.81645 LUMO: -0.85444 factor:1 | 1 (-0.00433) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.11796 HOMO: -6.20692 LUMO: 1.30887 factor:1 | -1 (0.45604) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03003 HOMO: -5.96201 LUMO: 1.33880 factor:1 | 1 (-0.45604) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.72003 HOMO: -6.52529 LUMO: 1.58914 factor:1 | 1 (-1.14603) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21200 HOMO: -6.58516 LUMO: 1.97555 factor:1 | 1 (-0.63800) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15099 HOMO: -6.84366 LUMO: 0.15783 factor:1 | 1 (-0.57699) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.68130 HOMO: -6.45726 LUMO: 0.42994 factor:1 | -1 (0.89270) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80448 HOMO: -6.75387 LUMO: 0.14422 factor:1 | 1 (-0.23048) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.95290 HOMO: -6.69944 LUMO: 1.79051 factor:1 | -1 (0.62110) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.82928 HOMO: -6.59876 LUMO: 1.90208 factor:1 | -1 (0.74472) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12704 HOMO: -7.05863 LUMO: 1.20819 factor:1 | 1 (-0.55304) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30122 HOMO: -6.54978 LUMO: 2.01636 factor:1 | 1 (-0.72722) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49312 HOMO: -5.52119 LUMO: 1.95106 factor:1 | 1 (-0.91912) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.21710 HOMO: -6.53617 LUMO: 1.60275 factor:1 | 1 (-1.64311) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.56858 HOMO: -6.11440 LUMO: 1.89119 factor:1 | 1 (-0.99458) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93552 HOMO: -7.31986 LUMO: 0.48708 factor:1 | 1 (-1.36152) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99948 HOMO: -6.76475 LUMO: -0.75648 factor:1 | 1 (-0.42548) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.45899 HOMO: -6.76747 LUMO: -1.06941 factor:1 | 1 (-1.88499) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76233 HOMO: -6.87087 LUMO: 0.72927 factor:1 | 1 (-0.18833) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31064 HOMO: -7.00965 LUMO: 0.02177 factor:1 | 1 (-0.73664) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12182 HOMO: -6.54706 LUMO: -0.03265 factor:1 | 1 (-0.54782) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.02687 HOMO: -6.62325 LUMO: -0.63675 factor:1 | 1 (-1.45287) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08233 HOMO: -7.03414 LUMO: -1.24084 factor:1 | 1 (-1.50833) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66752 HOMO: -7.04503 LUMO: -0.10068 factor:1 | 1 (-0.09353) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13983 HOMO: -6.67223 LUMO: 0.03537 factor:1 | 1 (-0.56583) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.63785 HOMO: -6.82734 LUMO: 0.58777 factor:1 | 1 (-2.06385) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82388 HOMO: -6.84366 LUMO: 0.46531 factor:1 | 1 (-0.24988) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06881 HOMO: -7.03959 LUMO: -1.15104 factor:1 | 1 (-0.49481) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28340 HOMO: -6.91169 LUMO: -0.41361 factor:1 | 1 (-0.70940) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17993 HOMO: -7.10217 LUMO: -0.44627 factor:1 | 1 (-1.60593) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.02346 HOMO: -6.88176 LUMO: -0.19592 factor:1 | -1 (0.55054) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.83799 HOMO: -7.21374 LUMO: -0.46531 factor:1 | -1 (0.73601) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.64160 HOMO: -6.54978 LUMO: 0.16871 factor:1 | -1 (0.93240) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.74635 HOMO: -6.71305 LUMO: -0.13061 factor:1 | -1 (1.82765) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79651 HOMO: -6.74842 LUMO: -0.36191 factor:1 | 1 (-0.22251) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63996 HOMO: -6.74570 LUMO: -0.09796 factor:1 | 1 (-0.06596) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97888 HOMO: -6.93890 LUMO: -0.27211 factor:1 | 1 (-0.40488) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63999 HOMO: -6.88720 LUMO: -0.18776 factor:1 | 1 (-0.06599) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71196 HOMO: -6.74842 LUMO: 0.02993 factor:1 | 1 (-0.13796) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61735 HOMO: -6.70216 LUMO: 0.01361 factor:1 | 1 (-0.04335) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.31114 HOMO: -6.90625 LUMO: 0.00544 factor:1 | -1 (0.26286) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.09859 HOMO: -6.18243 LUMO: 0.25851 factor:1 | -1 (0.47541) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.07990 HOMO: -6.32937 LUMO: -0.20953 factor:1 | 1 (-1.50591) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.96785 HOMO: -6.78108 LUMO: 0.00544 factor:1 | 1 (-1.39385) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.30638 HOMO: -5.97562 LUMO: 0.28572 factor:1 | 1 (-1.73239) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.81740 HOMO: -5.97290 LUMO: -0.18504 factor:1 | 1 (-1.24340) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.80174 HOMO: -6.12800 LUMO: 0.42178 factor:1 | -1 (0.77226) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.43047 HOMO: -6.24229 LUMO: -0.00816 factor:1 | -1 (1.14353) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.03184 HOMO: -6.61781 LUMO: 0.12789 factor:1 | -1 (0.54216) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.66664 HOMO: -6.70489 LUMO: 0.14694 factor:1 | -1 (1.90735) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.64898 HOMO: -6.86543 LUMO: -0.21225 factor:1 | -1 (0.92502) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55381 HOMO: -6.90081 LUMO: -0.20136 factor:1 | -1 (0.02019) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45655 HOMO: -7.12938 LUMO: -0.25851 factor:1 | -1 (0.11744) | 1 | 1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70366 HOMO: -6.93074 LUMO: -0.26667 factor:1 | 1 (-0.12966) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.90430 HOMO: -7.00421 LUMO: -0.31021 factor:1 | -1 (0.66970) | -1 | -1 |
| G: -5684.20830 HOMO: -8.44097 LUMO: -1.47758 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.33587 HOMO: -7.10761 LUMO: -0.17415 factor:1 | -1 (0.23813) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65399 HOMO: -8.21240 LUMO: 0.05987 factor:1 | 1 (-1.07999) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.30018 HOMO: -7.14843 LUMO: -0.46531 factor:1 | 1 (-1.72618) | 1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00798 HOMO: -6.80829 LUMO: -0.29933 factor:1 | 1 (-1.43399) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.26304 HOMO: -6.84094 LUMO: -0.53606 factor:1 | 1 (-1.68904) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47059 HOMO: -6.81917 LUMO: -0.26667 factor:1 | 1 (-0.89659) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09393 HOMO: -6.85727 LUMO: -1.20002 factor:1 | 1 (-0.51993) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43793 HOMO: -6.39468 LUMO: -1.06941 factor:1 | 1 (-0.86393) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97084 HOMO: -6.00827 LUMO: -1.94017 factor:1 | 1 (-1.39684) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79572 HOMO: -6.80829 LUMO: 0.18504 factor:1 | 1 (-0.22172) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.40853 HOMO: -6.54434 LUMO: -0.95784 factor:1 | -1 (0.16547) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.46445 HOMO: -6.45454 LUMO: -0.07347 factor:1 | -1 (0.10955) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51095 HOMO: -5.33887 LUMO: 1.11839 factor:1 | -1 (0.06305) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50461 HOMO: -5.75249 LUMO: 0.70477 factor:1 | -1 (0.06939) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.31682 HOMO: -5.64092 LUMO: 0.87076 factor:1 | -1 (0.25717) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94486 HOMO: -5.14295 LUMO: 1.06124 factor:1 | 1 (-0.37086) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.93252 HOMO: -5.05043 LUMO: 1.21091 factor:1 | -1 (0.64148) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.95352 HOMO: -5.05588 LUMO: 1.02859 factor:1 | -1 (0.62047) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.93513 HOMO: -5.76337 LUMO: 0.79457 factor:1 | -1 (0.63887) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.58235 HOMO: -5.01506 LUMO: 1.00138 factor:1 | 1 (-0.00835) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94513 HOMO: -4.84363 LUMO: 1.53744 factor:1 | 1 (-1.37113) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.37262 HOMO: -5.17833 LUMO: 1.45309 factor:1 | 1 (-1.79862) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99435 HOMO: -5.13751 LUMO: 0.51157 factor:1 | 1 (-1.42035) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.36113 HOMO: -5.56473 LUMO: 0.32109 factor:1 | 1 (-1.78713) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65965 HOMO: -4.69941 LUMO: 1.14016 factor:1 | 1 (-1.08565) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.86286 HOMO: -4.49260 LUMO: 1.86398 factor:1 | 1 (-2.28886) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.32663 HOMO: -4.32117 LUMO: 1.68438 factor:1 | 1 (-1.75263) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06586 HOMO: -4.44906 LUMO: 1.37690 factor:1 | 1 (-1.49186) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00015 HOMO: -4.62049 LUMO: 1.34968 factor:1 | 1 (-1.42615) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70822 HOMO: -4.59600 LUMO: 1.58370 factor:1 | 1 (-1.13422) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.48378 HOMO: -4.98785 LUMO: 1.46669 factor:1 | 1 (-1.90978) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78499 HOMO: -5.06676 LUMO: 1.27349 factor:1 | 1 (-1.21099) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.04711 HOMO: -5.09125 LUMO: 1.13471 factor:1 | 1 (-1.47312) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98405 HOMO: -4.84635 LUMO: 1.33608 factor:1 | 1 (-0.41005) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92864 HOMO: -4.94431 LUMO: 1.18370 factor:1 | 1 (-0.35465) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94132 HOMO: -4.92526 LUMO: 1.39867 factor:1 | 1 (-1.36732) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.70470 HOMO: -5.71983 LUMO: 0.60137 factor:1 | 1 (-2.13071) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93232 HOMO: -5.10486 LUMO: 1.05580 factor:1 | 1 (-0.35832) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.40542 HOMO: -5.20282 LUMO: 1.01226 factor:1 | 1 (-0.83142) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.63113 HOMO: -4.98513 LUMO: 1.53744 factor:1 | 1 (-2.05713) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35507 HOMO: -5.67085 LUMO: 0.17687 factor:1 | 1 (-0.78108) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00432 HOMO: -5.87222 LUMO: 0.12517 factor:1 | 1 (-0.43032) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19820 HOMO: -5.20826 LUMO: 0.91702 factor:1 | 1 (-0.62420) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66523 HOMO: -5.94569 LUMO: 0.63130 factor:1 | 1 (-1.09123) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62270 HOMO: -5.35792 LUMO: 0.91430 factor:1 | 1 (-1.04870) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48479 HOMO: -5.36336 LUMO: 1.44220 factor:1 | 1 (-0.91079) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.71967 HOMO: -5.83412 LUMO: 0.71294 factor:1 | 1 (-2.14567) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62937 HOMO: -4.97696 LUMO: 1.72792 factor:1 | 1 (-0.05538) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42806 HOMO: -5.55929 LUMO: 0.23130 factor:1 | 1 (-0.85406) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.62862 HOMO: -5.71167 LUMO: 0.47348 factor:1 | 1 (-2.05462) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.58687 HOMO: -7.31986 LUMO: -2.54699 factor:1 | 1 (-0.01287) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36680 HOMO: -5.34704 LUMO: 1.19730 factor:1 | 1 (-0.79280) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95714 HOMO: -5.45860 LUMO: 0.80818 factor:1 | 1 (-0.38314) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80823 HOMO: -5.12663 LUMO: 1.20274 factor:1 | 1 (-1.23423) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.99548 HOMO: -5.37153 LUMO: 1.05580 factor:1 | -1 (0.57851) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70725 HOMO: -5.47221 LUMO: 0.97961 factor:1 | 1 (-0.13325) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94855 HOMO: -5.06948 LUMO: 1.12111 factor:1 | 1 (-1.37456) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55774 HOMO: -5.19737 LUMO: 1.25444 factor:1 | 1 (-0.98375) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94651 HOMO: -5.27901 LUMO: 1.00682 factor:1 | 1 (-1.37252) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.52342 HOMO: -5.38513 LUMO: 0.49253 factor:1 | 1 (-1.94942) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92663 HOMO: -5.12390 LUMO: 1.22995 factor:1 | 1 (-0.35263) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51726 HOMO: -5.31438 LUMO: 0.70205 factor:1 | -1 (0.05674) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.96272 HOMO: -5.17561 LUMO: 1.04492 factor:1 | -1 (0.61128) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51152 HOMO: -4.94431 LUMO: 1.52656 factor:1 | -1 (0.06248) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.10509 HOMO: -5.13751 LUMO: 0.93879 factor:1 | -1 (0.46891) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.44791 HOMO: -5.49942 LUMO: 0.97689 factor:1 | -1 (1.12609) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55015 HOMO: -5.79058 LUMO: 0.53879 factor:1 | 1 (-0.97615) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.80287 HOMO: -5.36881 LUMO: 1.56465 factor:1 | 1 (-1.22887) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35843 HOMO: -4.67492 LUMO: 1.32792 factor:1 | -1 (0.21557) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28179 HOMO: -4.60145 LUMO: 1.19458 factor:1 | 1 (-0.70780) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77885 HOMO: -4.49260 LUMO: 1.60547 factor:1 | 1 (-0.20485) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.46423 HOMO: -4.65043 LUMO: 1.34696 factor:1 | -1 (0.10977) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.49846 HOMO: -4.77560 LUMO: 1.35241 factor:1 | -1 (0.07554) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81218 HOMO: -4.94431 LUMO: 1.17825 factor:1 | 1 (-0.23818) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69738 HOMO: -4.87084 LUMO: 1.41771 factor:1 | 1 (-0.12338) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.37729 HOMO: -5.34432 LUMO: 1.16737 factor:1 | -1 (0.19671) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35174 HOMO: -4.94975 LUMO: 1.67622 factor:1 | -1 (0.22226) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69792 HOMO: -4.81369 LUMO: 1.14288 factor:1 | 1 (-0.12392) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.36385 HOMO: -5.22459 LUMO: 0.29660 factor:1 | -1 (0.21015) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.28455 HOMO: -5.21642 LUMO: 0.37824 factor:1 | -1 (0.28945) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72627 HOMO: -5.00417 LUMO: 1.01226 factor:1 | 1 (-0.15227) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56880 HOMO: -5.46677 LUMO: 0.10612 factor:1 | -1 (0.00520) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38103 HOMO: -5.51303 LUMO: 0.54151 factor:1 | 1 (-0.80704) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.27507 HOMO: -5.63004 LUMO: 0.17960 factor:1 | 1 (-0.70107) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16770 HOMO: -4.79193 LUMO: 1.12111 factor:1 | 1 (-0.59370) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02291 HOMO: -5.43411 LUMO: 0.45987 factor:1 | 1 (-0.44891) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.95558 HOMO: -7.06135 LUMO: -2.13881 factor:1 | 1 (-1.38158) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98690 HOMO: -5.33071 LUMO: 1.14016 factor:1 | 1 (-0.41291) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06644 HOMO: -7.12394 LUMO: -0.03810 factor:1 | 1 (-0.49244) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03251 HOMO: -7.20558 LUMO: -2.50889 factor:1 | 1 (-0.45851) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09069 HOMO: -7.26816 LUMO: -2.11432 factor:1 | 1 (-0.51669) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94393 HOMO: -7.89674 LUMO: 0.31021 factor:1 | 1 (-1.36993) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81931 HOMO: -7.26544 LUMO: 0.22858 factor:1 | 1 (-0.24531) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71585 HOMO: -7.12666 LUMO: -0.02449 factor:1 | 1 (-0.14185) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63903 HOMO: -7.68722 LUMO: 0.71838 factor:1 | 1 (-1.06503) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61707 HOMO: -6.86271 LUMO: -0.96056 factor:1 | 1 (-0.04308) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61577 HOMO: -7.07496 LUMO: -1.11839 factor:1 | 1 (-0.04177) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.31938 HOMO: -7.06952 LUMO: -2.08439 factor:1 | -1 (0.25462) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.84523 HOMO: -6.60965 LUMO: -2.11977 factor:1 | -1 (1.72877) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81210 HOMO: -6.87360 LUMO: -1.85854 factor:1 | 1 (-0.23810) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61821 HOMO: -7.67089 LUMO: -0.24762 factor:1 | 1 (-1.04421) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.76918 HOMO: -6.45726 LUMO: -1.86398 factor:1 | 1 (-1.19518) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42082 HOMO: -6.91713 LUMO: 0.33198 factor:1 | 1 (-0.84682) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68499 HOMO: -6.83278 LUMO: 0.26667 factor:1 | 1 (-1.11099) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70670 HOMO: -6.89264 LUMO: -1.00682 factor:1 | 1 (-1.13270) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39859 HOMO: -6.57427 LUMO: 0.22041 factor:1 | 1 (-0.82459) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61456 HOMO: -7.52123 LUMO: -0.01905 factor:1 | 1 (-1.04056) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56252 HOMO: -7.37429 LUMO: -0.08980 factor:1 | -1 (0.01148) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.83948 HOMO: -7.28449 LUMO: -0.26395 factor:1 | -1 (0.73452) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.11961 HOMO: -6.79740 LUMO: -0.60954 factor:1 | 1 (-1.54561) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65560 HOMO: -7.12666 LUMO: -0.60681 factor:1 | 1 (-1.08160) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35831 HOMO: -6.96611 LUMO: -0.30477 factor:1 | 1 (-0.78431) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.41418 HOMO: -7.08040 LUMO: -0.31293 factor:1 | -1 (2.15982) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.23058 HOMO: -6.78924 LUMO: -0.73743 factor:1 | 1 (-0.65658) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05627 HOMO: -7.57293 LUMO: -1.11295 factor:1 | 1 (-0.48227) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22117 HOMO: -7.15932 LUMO: -0.23130 factor:1 | 1 (-0.64717) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84568 HOMO: -7.48585 LUMO: -0.10068 factor:1 | 1 (-0.27168) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96914 HOMO: -7.17020 LUMO: -0.26123 factor:1 | 1 (-0.39514) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.18012 HOMO: -7.43143 LUMO: -0.16055 factor:1 | -1 (1.39388) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78085 HOMO: -7.14843 LUMO: -0.10612 factor:1 | 1 (-1.20685) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00069 HOMO: -6.95523 LUMO: -0.22585 factor:1 | 1 (-1.42669) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67037 HOMO: -7.06680 LUMO: -0.51974 factor:1 | 1 (-1.09637) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50977 HOMO: -6.80829 LUMO: -0.64763 factor:1 | 1 (-0.93577) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69867 HOMO: -7.13210 LUMO: -0.48164 factor:1 | 1 (-1.12467) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36721 HOMO: -7.16204 LUMO: -0.45715 factor:1 | 1 (-0.79321) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61702 HOMO: -7.15115 LUMO: -0.43266 factor:1 | 1 (-0.04302) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78081 HOMO: -7.15932 LUMO: -2.52794 factor:1 | 1 (-0.20681) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.39993 HOMO: -7.21102 LUMO: -2.65311 factor:1 | -1 (0.17407) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87877 HOMO: -6.57427 LUMO: -2.78645 factor:1 | 1 (-0.30477) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.02692 HOMO: -6.40828 LUMO: -3.23815 factor:1 | -1 (1.54708) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52532 HOMO: -7.71987 LUMO: -0.20953 factor:1 | -1 (0.04868) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64369 HOMO: -7.47769 LUMO: -0.43810 factor:1 | 1 (-0.06969) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.33353 HOMO: -6.68040 LUMO: -2.22589 factor:1 | -1 (0.24047) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81974 HOMO: -6.92802 LUMO: -1.99187 factor:1 | 1 (-0.24575) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.93095 HOMO: -7.73620 LUMO: 0.01633 factor:1 | -1 (1.64305) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60218 HOMO: -7.28721 LUMO: -0.18504 factor:1 | 1 (-1.02818) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87501 HOMO: -7.49674 LUMO: -0.19864 factor:1 | 1 (-0.30101) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.20221 HOMO: -7.10489 LUMO: -2.56331 factor:1 | -1 (0.37179) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.37188 HOMO: -7.36612 LUMO: 0.16055 factor:1 | 1 (-1.79788) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70648 HOMO: -7.67633 LUMO: 0.33198 factor:1 | 1 (-1.13248) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41671 HOMO: -7.07768 LUMO: -0.27483 factor:1 | 1 (-0.84271) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47434 HOMO: -7.32531 LUMO: 0.05442 factor:1 | 1 (-0.90034) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50003 HOMO: -6.79740 LUMO: -1.21635 factor:1 | 1 (-0.92603) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.34261 HOMO: -7.14027 LUMO: 0.12517 factor:1 | 1 (-0.76861) | 1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.96752 HOMO: -7.17292 LUMO: 0.16871 factor:1 | 1 (-1.39352) | 1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94372 HOMO: -7.08312 LUMO: -1.38778 factor:1 | 1 (-0.36972) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72818 HOMO: -6.75387 LUMO: -1.88031 factor:1 | 1 (-0.15418) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63070 HOMO: -7.07768 LUMO: -1.25717 factor:1 | 1 (-1.05670) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10590 HOMO: -6.46543 LUMO: -1.14016 factor:1 | 1 (-0.53190) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05205 HOMO: -7.37973 LUMO: -0.45987 factor:1 | 1 (-0.47805) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43843 HOMO: -7.46408 LUMO: 0.03265 factor:1 | -1 (0.13557) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.58083 HOMO: -7.96477 LUMO: -0.19864 factor:1 | 1 (-0.00683) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.17347 HOMO: -6.93890 LUMO: -1.11839 factor:1 | -1 (0.40052) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00817 HOMO: -7.06408 LUMO: -1.08846 factor:1 | 1 (-1.43418) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98941 HOMO: -7.14027 LUMO: -0.33470 factor:1 | 1 (-0.41541) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.66356 HOMO: -7.38245 LUMO: 0.10885 factor:1 | 1 (-2.08956) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52019 HOMO: -7.59470 LUMO: -1.21363 factor:1 | 1 (-0.94619) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94807 HOMO: -7.23279 LUMO: -1.23812 factor:1 | 1 (-0.37407) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73984 HOMO: -6.90897 LUMO: 0.23402 factor:1 | 1 (-1.16584) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79359 HOMO: -7.36340 LUMO: -0.17143 factor:1 | 1 (-0.21960) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09365 HOMO: -6.61781 LUMO: -0.01361 factor:1 | 1 (-0.51966) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04897 HOMO: -6.80013 LUMO: 0.38368 factor:1 | 1 (-0.47497) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59263 HOMO: -6.72121 LUMO: -0.95512 factor:1 | 1 (-1.01863) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.27826 HOMO: -6.24773 LUMO: -0.69933 factor:1 | 1 (-0.70426) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.72862 HOMO: -6.56883 LUMO: 0.14694 factor:1 | -1 (0.84538) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54626 HOMO: -6.51441 LUMO: -1.27621 factor:1 | 1 (-0.97226) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.37380 HOMO: -6.91986 LUMO: -1.16737 factor:1 | 1 (-0.79980) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81902 HOMO: -6.17971 LUMO: -0.65307 factor:1 | -1 (0.75498) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38877 HOMO: -7.22462 LUMO: 0.04354 factor:1 | -1 (0.18523) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60075 HOMO: -7.16204 LUMO: -0.23674 factor:1 | 1 (-0.02675) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.41337 HOMO: -6.81645 LUMO: -0.19320 factor:1 | -1 (0.16063) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05940 HOMO: -6.69400 LUMO: 0.04082 factor:1 | 1 (-0.48540) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15883 HOMO: -6.63141 LUMO: -0.22858 factor:1 | -1 (0.41516) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.30600 HOMO: -6.92258 LUMO: -1.11295 factor:1 | 1 (-1.73200) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42242 HOMO: -6.60148 LUMO: -1.13744 factor:1 | 1 (-0.84842) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70910 HOMO: -6.78108 LUMO: -0.82450 factor:1 | 1 (-0.13510) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.91548 HOMO: -7.05591 LUMO: -0.97145 factor:1 | -1 (0.65852) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60779 HOMO: -6.65318 LUMO: -1.26261 factor:1 | 1 (-1.03379) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.79521 HOMO: -6.98244 LUMO: -0.98233 factor:1 | -1 (0.77879) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38005 HOMO: -7.11850 LUMO: -0.99594 factor:1 | 1 (-0.80606) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43603 HOMO: -6.64230 LUMO: -0.93879 factor:1 | 1 (-0.86203) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62972 HOMO: -6.62053 LUMO: -1.22451 factor:1 | 1 (-1.05572) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.66081 HOMO: -7.02598 LUMO: -0.85172 factor:1 | -1 (0.91319) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.18431 HOMO: -7.06680 LUMO: -0.89253 factor:1 | 1 (-1.61032) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.40310 HOMO: -7.17292 LUMO: 0.00272 factor:1 | 1 (-0.82910) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35412 HOMO: -7.03142 LUMO: -0.35103 factor:1 | 1 (-0.78012) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47394 HOMO: -6.96884 LUMO: -0.09796 factor:1 | -1 (0.10006) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.54337 HOMO: -6.56339 LUMO: -0.99322 factor:1 | -1 (1.03063) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.63470 HOMO: -7.08857 LUMO: -0.17687 factor:1 | 1 (-1.06070) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68499 HOMO: -7.05863 LUMO: -0.22041 factor:1 | 1 (-0.11100) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.82696 HOMO: -7.15115 LUMO: -0.17960 factor:1 | -1 (0.74703) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.66470 HOMO: -6.67495 LUMO: -0.96600 factor:1 | -1 (0.90930) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79974 HOMO: -6.74026 LUMO: -1.79867 factor:1 | 1 (-0.22575) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82364 HOMO: -6.73482 LUMO: -1.78235 factor:1 | 1 (-0.24964) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52804 HOMO: -6.09807 LUMO: 0.16871 factor:1 | -1 (0.04596) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90935 HOMO: -6.72393 LUMO: 0.27211 factor:1 | 1 (-0.33535) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01420 HOMO: -6.40556 LUMO: -0.04354 factor:1 | 1 (-0.44020) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97577 HOMO: -6.56883 LUMO: 0.22041 factor:1 | 1 (-0.40178) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61201 HOMO: -7.22462 LUMO: 0.15783 factor:1 | 1 (-0.03801) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.82956 HOMO: -6.83550 LUMO: 0.19320 factor:1 | -1 (1.74444) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.92657 HOMO: -7.26816 LUMO: -0.07619 factor:1 | -1 (1.64743) | 1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.77950 HOMO: -7.13483 LUMO: 0.33198 factor:1 | -1 (2.79450) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.68758 HOMO: -6.58243 LUMO: -0.26395 factor:1 | -1 (2.88642) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.90478 HOMO: -7.38517 LUMO: 0.17143 factor:1 | -1 (2.66922) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48442 HOMO: -6.80013 LUMO: 0.25851 factor:1 | -1 (0.08958) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.09282 HOMO: -6.96611 LUMO: 0.11429 factor:1 | -1 (0.48118) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64216 HOMO: -6.51713 LUMO: -1.14560 factor:1 | 1 (-0.06816) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.02915 HOMO: -7.15387 LUMO: -0.35647 factor:1 | -1 (0.54485) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74480 HOMO: -5.26540 LUMO: 1.26805 factor:1 | 1 (-0.17081) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.10787 HOMO: -6.76475 LUMO: -0.16327 factor:1 | -1 (0.46613) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50153 HOMO: -6.55250 LUMO: -0.71838 factor:1 | -1 (0.07246) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.84356 HOMO: -6.76203 LUMO: -1.08301 factor:1 | -1 (0.73044) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.23177 HOMO: -7.14027 LUMO: -0.01633 factor:1 | -1 (1.34223) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.46260 HOMO: -6.94979 LUMO: -0.93879 factor:1 | -1 (1.11139) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.97206 HOMO: -6.74842 LUMO: 0.31293 factor:1 | -1 (1.60193) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.24995 HOMO: -6.43821 LUMO: 0.05987 factor:1 | -1 (1.32405) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.36082 HOMO: -6.60420 LUMO: 0.22585 factor:1 | -1 (0.21317) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.03505 HOMO: -6.43821 LUMO: 0.05987 factor:1 | -1 (0.53895) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15522 HOMO: -6.34570 LUMO: 1.43948 factor:1 | -1 (0.41878) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35623 HOMO: -6.03004 LUMO: 1.21363 factor:1 | -1 (0.21777) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.07198 HOMO: -6.68040 LUMO: -0.92247 factor:1 | -1 (0.50202) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.12482 HOMO: -6.92530 LUMO: -0.31293 factor:1 | -1 (0.44918) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.69224 HOMO: -6.94979 LUMO: -0.19864 factor:1 | -1 (0.88176) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65131 HOMO: -6.80829 LUMO: -0.30477 factor:1 | 1 (-0.07731) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71917 HOMO: -7.22734 LUMO: -1.02859 factor:1 | 1 (-0.14517) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43536 HOMO: -6.93890 LUMO: -0.72382 factor:1 | -1 (0.13864) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.08262 HOMO: -7.27088 LUMO: -0.78097 factor:1 | -1 (0.49138) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.14668 HOMO: -7.29809 LUMO: -0.97145 factor:1 | 1 (-1.57268) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.68019 HOMO: -7.18925 LUMO: -0.94696 factor:1 | 1 (-2.10619) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.15563 HOMO: -7.33891 LUMO: -0.96873 factor:1 | 1 (-1.58163) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78077 HOMO: -7.36068 LUMO: -0.28028 factor:1 | 1 (-1.20677) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.26603 HOMO: -7.10761 LUMO: -1.14832 factor:1 | 1 (-1.69203) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66069 HOMO: -6.94707 LUMO: -0.65307 factor:1 | 1 (-1.08669) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52419 HOMO: -6.91713 LUMO: -1.81228 factor:1 | 1 (-0.95019) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92312 HOMO: -6.78652 LUMO: -2.01636 factor:1 | 1 (-0.34912) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05921 HOMO: -6.52801 LUMO: -1.17553 factor:1 | 1 (-0.48521) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97909 HOMO: -7.54844 LUMO: -1.18642 factor:1 | 1 (-0.40510) | 1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79183 HOMO: -7.52939 LUMO: -1.23812 factor:1 | 1 (-0.21783) | 1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96130 HOMO: -7.94572 LUMO: -0.81634 factor:1 | 1 (-0.38730) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93137 HOMO: -7.55932 LUMO: -0.86260 factor:1 | 1 (-0.35737) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.49468 HOMO: -7.72259 LUMO: -1.39050 factor:1 | -1 (0.07932) | 1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90753 HOMO: -7.11850 LUMO: -1.01498 factor:1 | 1 (-0.33353) | 1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83501 HOMO: -7.09673 LUMO: -1.00954 factor:1 | 1 (-0.26101) | 1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97977 HOMO: -6.06270 LUMO: 0.16327 factor:1 | 1 (-1.40577) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63245 HOMO: -5.71167 LUMO: 0.70477 factor:1 | 1 (-0.05845) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93055 HOMO: -5.38241 LUMO: 0.86260 factor:1 | 1 (-0.35655) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78102 HOMO: -5.67357 LUMO: 1.27621 factor:1 | 1 (-0.20702) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.42450 HOMO: -7.56204 LUMO: -0.68573 factor:1 | -1 (0.14950) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07395 HOMO: -5.57833 LUMO: 1.13199 factor:1 | 1 (-0.49995) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.11737 HOMO: -7.58653 LUMO: -0.66124 factor:1 | -1 (1.45663) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.75875 HOMO: -7.91851 LUMO: -1.10206 factor:1 | -1 (1.81524) | 1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.70403 HOMO: -6.48992 LUMO: -1.00138 factor:1 | -1 (1.86997) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.42688 HOMO: -7.09673 LUMO: -0.45171 factor:1 | -1 (2.14711) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.53550 HOMO: -6.63686 LUMO: 0.09252 factor:1 | -1 (1.03850) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.70372 HOMO: -6.84366 LUMO: -0.14422 factor:1 | -1 (0.87027) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95297 HOMO: -6.93074 LUMO: 0.04354 factor:1 | 1 (-0.37897) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45114 HOMO: -6.90353 LUMO: -0.19864 factor:1 | -1 (0.12286) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81906 HOMO: -6.59876 LUMO: -0.10068 factor:1 | 1 (-0.24507) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.41397 HOMO: -6.74570 LUMO: -0.44627 factor:1 | -1 (0.16003) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81487 HOMO: -6.60148 LUMO: -0.61770 factor:1 | 1 (-0.24088) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59503 HOMO: -6.55794 LUMO: -1.06941 factor:1 | 1 (-0.02103) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.46640 HOMO: -7.12666 LUMO: -0.11973 factor:1 | 1 (-0.89240) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06554 HOMO: -7.21646 LUMO: -0.50069 factor:1 | 1 (-1.49154) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91697 HOMO: -7.27632 LUMO: -1.00682 factor:1 | 1 (-0.34297) | 1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66826 HOMO: -6.74298 LUMO: 0.04354 factor:1 | 1 (-0.09426) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91281 HOMO: -6.37291 LUMO: 0.14150 factor:1 | 1 (-0.33881) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72355 HOMO: -5.61371 LUMO: 1.28438 factor:1 | 1 (-0.14955) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53680 HOMO: -5.52119 LUMO: 0.99866 factor:1 | -1 (0.03720) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80935 HOMO: -6.51985 LUMO: -0.10885 factor:1 | 1 (-0.23535) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.06684 HOMO: -5.61371 LUMO: 0.77280 factor:1 | -1 (1.50716) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92347 HOMO: -5.58922 LUMO: 0.24490 factor:1 | 1 (-0.34948) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84236 HOMO: -6.32665 LUMO: -0.57144 factor:1 | 1 (-0.26836) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67650 HOMO: -6.29127 LUMO: -0.93607 factor:1 | 1 (-0.10251) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71163 HOMO: -5.49670 LUMO: 0.27211 factor:1 | 1 (-0.13764) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75811 HOMO: -5.68990 LUMO: 0.24218 factor:1 | 1 (-0.18411) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66918 HOMO: -5.68174 LUMO: 0.69933 factor:1 | 1 (-0.09519) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.37302 HOMO: -5.28173 LUMO: 1.00954 factor:1 | -1 (0.20098) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67917 HOMO: -5.94025 LUMO: 0.73471 factor:1 | 1 (-0.10517) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.00415 HOMO: -5.65725 LUMO: 1.28710 factor:1 | -1 (1.56985) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22985 HOMO: -5.41507 LUMO: 0.87076 factor:1 | 1 (-0.65585) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96900 HOMO: -5.96474 LUMO: 0.29660 factor:1 | 1 (-0.39500) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.41741 HOMO: -7.00421 LUMO: 0.08708 factor:1 | -1 (1.15659) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.40780 HOMO: -5.40418 LUMO: 0.90070 factor:1 | -1 (1.16620) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.68587 HOMO: -7.00421 LUMO: -0.30477 factor:1 | -1 (0.88813) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.71695 HOMO: -5.85861 LUMO: 0.74015 factor:1 | -1 (0.85705) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.65423 HOMO: -5.71439 LUMO: 0.26395 factor:1 | -1 (0.91977) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79576 HOMO: -7.13755 LUMO: -0.78369 factor:1 | 1 (-1.22176) | 1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38197 HOMO: -7.31442 LUMO: -0.98233 factor:1 | -1 (0.19203) | 1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79811 HOMO: -7.25728 LUMO: -1.00410 factor:1 | 1 (-0.22411) | 1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.96396 HOMO: -7.48585 LUMO: -0.83811 factor:1 | 1 (-1.38996) | 1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.27684 HOMO: -7.24911 LUMO: -0.77280 factor:1 | 1 (-0.70284) | 1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24601 HOMO: -7.55116 LUMO: -1.19730 factor:1 | 1 (-0.67201) | 1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00043 HOMO: -5.76881 LUMO: 0.28028 factor:1 | 1 (-0.42643) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70565 HOMO: -5.77153 LUMO: -0.26939 factor:1 | 1 (-0.13165) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76962 HOMO: -5.82868 LUMO: 0.36735 factor:1 | 1 (-0.19562) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85240 HOMO: -5.83140 LUMO: -0.17960 factor:1 | 1 (-0.27840) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71754 HOMO: -6.28855 LUMO: 0.01088 factor:1 | 1 (-0.14354) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53237 HOMO: -6.31576 LUMO: 0.25307 factor:1 | -1 (0.04163) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90206 HOMO: -7.06408 LUMO: -2.76196 factor:1 | 1 (-0.32806) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.03016 HOMO: -5.95657 LUMO: 0.37552 factor:1 | -1 (1.54384) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73394 HOMO: -6.61781 LUMO: 0.02721 factor:1 | 1 (-1.15994) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.40171 HOMO: -6.26678 LUMO: -0.66668 factor:1 | 1 (-0.82772) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50830 HOMO: -6.00011 LUMO: -0.13334 factor:1 | 1 (-0.93430) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41905 HOMO: -5.60555 LUMO: 0.67484 factor:1 | 1 (-0.84505) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07823 HOMO: -5.79875 LUMO: 0.99049 factor:1 | 1 (-0.50423) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44221 HOMO: -5.97834 LUMO: 0.48436 factor:1 | 1 (-0.86821) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38188 HOMO: -5.82868 LUMO: 0.91974 factor:1 | 1 (-0.80788) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.80459 HOMO: -5.86677 LUMO: 0.99594 factor:1 | -1 (2.76941) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.93958 HOMO: -5.70079 LUMO: 0.48980 factor:1 | -1 (2.63442) | -1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.70546 HOMO: -7.39605 LUMO: -1.02315 factor:1 | -1 (2.86854) | 1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.99104 HOMO: -7.22734 LUMO: -1.12927 factor:1 | -1 (2.58296) | 1 | -1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.21638 HOMO: -7.58926 LUMO: -0.65035 factor:1 | -1 (2.35762) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.94758 HOMO: -7.43959 LUMO: -0.75648 factor:1 | -1 (2.62642) | 1 | 1 |
| G: -5684.20830 HOMO: -10.05733 LUMO: -2.51977 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71648 HOMO: -7.55388 LUMO: -1.15104 factor:1 | 1 (-0.14248) | 1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.18126 HOMO: -6.74570 LUMO: -2.85447 factor:1 | -1 (0.39274) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.14708 HOMO: -7.35524 LUMO: -1.25444 factor:1 | -1 (0.42692) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78157 HOMO: -6.81645 LUMO: -1.20819 factor:1 | 1 (-0.20757) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.17911 HOMO: -6.99605 LUMO: -1.62996 factor:1 | -1 (0.39489) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.98150 HOMO: -6.88992 LUMO: -0.47620 factor:1 | -1 (0.59250) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67754 HOMO: -7.22190 LUMO: -0.01905 factor:1 | 1 (-0.10354) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29971 HOMO: -6.77836 LUMO: -0.82995 factor:1 | -1 (0.27429) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43345 HOMO: -6.48447 LUMO: -0.95512 factor:1 | -1 (0.14055) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81970 HOMO: -7.81239 LUMO: 1.22179 factor:1 | -1 (0.75430) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.35865 HOMO: -7.36612 LUMO: 0.19320 factor:1 | -1 (3.21535) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.79417 HOMO: -7.24095 LUMO: 0.33470 factor:1 | -1 (2.77983) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.93501 HOMO: -7.15932 LUMO: -2.24222 factor:1 | -1 (2.63899) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.73108 HOMO: -6.88992 LUMO: -2.69937 factor:1 | -1 (1.84292) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.20899 HOMO: -6.97428 LUMO: -0.98233 factor:1 | -1 (1.36500) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.90251 HOMO: -7.17564 LUMO: -0.93879 factor:1 | -1 (1.67149) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.46269 HOMO: -6.81645 LUMO: -1.14288 factor:1 | -1 (2.11130) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.40237 HOMO: -6.83006 LUMO: -0.63403 factor:1 | -1 (2.17163) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.74520 HOMO: -7.17292 LUMO: -1.07213 factor:1 | -1 (1.82880) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.48229 HOMO: -7.53755 LUMO: 0.15510 factor:1 | -1 (2.09171) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.38242 HOMO: -6.50080 LUMO: -0.51702 factor:1 | -1 (2.19158) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.51562 HOMO: -6.72665 LUMO: -0.80001 factor:1 | -1 (2.05838) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.77195 HOMO: -6.72665 LUMO: 1.68711 factor:1 | -1 (1.80205) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.04932 HOMO: -7.11850 LUMO: -0.75103 factor:1 | -1 (1.52468) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.05816 HOMO: -6.87087 LUMO: -0.85988 factor:1 | -1 (1.51584) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.46252 HOMO: -7.08857 LUMO: -0.89798 factor:1 | -1 (1.11148) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.34524 HOMO: -6.71305 LUMO: -0.85444 factor:1 | -1 (1.22876) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82323 HOMO: -6.59332 LUMO: -0.60137 factor:1 | 1 (-0.24923) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79928 HOMO: -7.28993 LUMO: 0.03265 factor:1 | 1 (-0.22528) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.18009 HOMO: -7.32258 LUMO: 0.13878 factor:1 | -1 (0.39391) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75207 HOMO: -7.28993 LUMO: 0.11429 factor:1 | 1 (-0.17807) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53914 HOMO: -6.86271 LUMO: -1.03947 factor:1 | -1 (0.03486) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88742 HOMO: -6.55794 LUMO: -0.84900 factor:1 | 1 (-0.31342) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29769 HOMO: -7.03686 LUMO: 0.11429 factor:1 | -1 (0.27630) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.97301 HOMO: -7.06952 LUMO: -0.96056 factor:1 | -1 (0.60099) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.49997 HOMO: -6.90897 LUMO: -0.99866 factor:1 | -1 (1.07403) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.15947 HOMO: -7.00693 LUMO: -0.83539 factor:1 | -1 (1.41453) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74233 HOMO: -6.74298 LUMO: -0.85172 factor:1 | 1 (-0.16833) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15736 HOMO: -6.83822 LUMO: -1.07213 factor:1 | 1 (-0.58336) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.89351 HOMO: -7.21918 LUMO: -1.55377 factor:1 | -1 (1.68049) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.98745 HOMO: -6.84094 LUMO: -1.09934 factor:1 | -1 (2.58655) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.86638 HOMO: -7.09129 LUMO: -0.85988 factor:1 | -1 (2.70761) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.63089 HOMO: -6.57971 LUMO: -2.27215 factor:1 | -1 (1.94311) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.48560 HOMO: -6.81373 LUMO: -1.86942 factor:1 | -1 (1.08840) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.63252 HOMO: -6.59060 LUMO: -2.30480 factor:1 | -1 (1.94148) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74984 HOMO: -6.72938 LUMO: -1.23540 factor:1 | 1 (-0.17584) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11521 HOMO: -6.94707 LUMO: -2.62318 factor:1 | 1 (-0.54121) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95055 HOMO: -7.28177 LUMO: -0.09796 factor:1 | 1 (-0.37655) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44581 HOMO: -6.80013 LUMO: -0.79729 factor:1 | -1 (0.12819) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.03709 HOMO: -7.26544 LUMO: 0.12789 factor:1 | -1 (0.53691) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21951 HOMO: -6.51713 LUMO: -0.49253 factor:1 | 1 (-0.64551) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76119 HOMO: -6.68856 LUMO: -0.77280 factor:1 | 1 (-0.18719) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.28531 HOMO: -6.41100 LUMO: -0.70750 factor:1 | -1 (0.28869) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78157 HOMO: -7.56204 LUMO: 0.22041 factor:1 | 1 (-0.20757) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.45844 HOMO: -6.68312 LUMO: 1.30343 factor:1 | -1 (1.11556) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.64636 HOMO: -7.24367 LUMO: 0.17415 factor:1 | -1 (0.92764) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.30119 HOMO: -7.52395 LUMO: 1.16737 factor:1 | -1 (1.27281) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.29983 HOMO: -6.89264 LUMO: 0.23130 factor:1 | -1 (1.27417) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.49402 HOMO: -7.21102 LUMO: 0.19048 factor:1 | -1 (0.07997) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85033 HOMO: -7.08312 LUMO: 0.25034 factor:1 | 1 (-0.27633) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.30959 HOMO: -6.49536 LUMO: -0.65852 factor:1 | -1 (0.26441) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.46085 HOMO: -6.85455 LUMO: 0.13606 factor:1 | -1 (0.11314) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09961 HOMO: -7.10217 LUMO: 0.35919 factor:1 | 1 (-0.52562) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29231 HOMO: -7.77429 LUMO: 1.19186 factor:1 | -1 (0.28169) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85332 HOMO: -6.57427 LUMO: -0.50069 factor:1 | 1 (-0.27932) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.89351 HOMO: -7.36340 LUMO: 0.10068 factor:1 | -1 (1.68049) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.88063 HOMO: -7.28177 LUMO: 0.15238 factor:1 | -1 (1.69336) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.57720 HOMO: -6.86543 LUMO: -0.84355 factor:1 | -1 (1.99680) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.83037 HOMO: -6.55794 LUMO: 1.39594 factor:1 | -1 (1.74362) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.87642 HOMO: -6.26134 LUMO: 1.53744 factor:1 | -1 (1.69758) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92470 HOMO: -5.97562 LUMO: 1.42316 factor:1 | 1 (-0.35070) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.28700 HOMO: -6.65046 LUMO: 1.44492 factor:1 | -1 (0.28700) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35742 HOMO: -6.92258 LUMO: 0.17415 factor:1 | -1 (0.21658) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90396 HOMO: -7.40966 LUMO: 0.19592 factor:1 | 1 (-0.32997) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77335 HOMO: -7.17564 LUMO: 0.16871 factor:1 | 1 (-0.19935) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.17799 HOMO: -7.46953 LUMO: 0.22313 factor:1 | -1 (0.39601) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59857 HOMO: -6.13345 LUMO: 1.85854 factor:1 | 1 (-0.02457) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.03140 HOMO: -6.99333 LUMO: -1.65717 factor:1 | -1 (0.54260) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96432 HOMO: -6.93074 LUMO: -1.79323 factor:1 | 1 (-0.39032) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.55673 HOMO: -6.87904 LUMO: -1.79323 factor:1 | -1 (1.01727) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.11181 HOMO: -6.84094 LUMO: 0.66940 factor:1 | -1 (0.46219) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.08909 HOMO: -7.13210 LUMO: -1.17553 factor:1 | -1 (0.48491) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50515 HOMO: -6.52801 LUMO: -2.23678 factor:1 | -1 (0.06884) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.49318 HOMO: -6.81917 LUMO: -1.86398 factor:1 | -1 (0.08082) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19862 HOMO: -7.30626 LUMO: -1.66806 factor:1 | -1 (0.37538) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62671 HOMO: -6.98516 LUMO: -1.40683 factor:1 | 1 (-0.05271) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68632 HOMO: -6.95523 LUMO: -0.97145 factor:1 | 1 (-1.11232) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79625 HOMO: -6.83278 LUMO: -2.68848 factor:1 | 1 (-1.22225) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11491 HOMO: -7.25456 LUMO: -2.97420 factor:1 | 1 (-0.54091) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66235 HOMO: -6.80557 LUMO: -2.65039 factor:1 | 1 (-1.08835) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79281 HOMO: -7.10489 LUMO: 0.77008 factor:1 | 1 (-0.21881) | 1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50961 HOMO: -7.28993 LUMO: -1.06124 factor:1 | 1 (-0.93561) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05284 HOMO: -7.11578 LUMO: -1.10206 factor:1 | 1 (-0.47884) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94865 HOMO: -6.91713 LUMO: -1.36329 factor:1 | 1 (-0.37465) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.75650 HOMO: -7.07224 LUMO: 0.51974 factor:1 | 1 (-1.18250) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10195 HOMO: -7.22734 LUMO: -0.93335 factor:1 | 1 (-0.52796) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14832 HOMO: -7.19469 LUMO: -0.96600 factor:1 | 1 (-0.57432) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.12830 HOMO: -6.93890 LUMO: -0.66940 factor:1 | -1 (0.44570) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19720 HOMO: -7.09673 LUMO: -1.05852 factor:1 | -1 (0.37680) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.21162 HOMO: -7.19197 LUMO: -2.26943 factor:1 | -1 (0.36237) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65958 HOMO: -6.90081 LUMO: -2.64767 factor:1 | 1 (-0.08558) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.32423 HOMO: -6.93890 LUMO: -2.65039 factor:1 | -1 (0.24977) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13494 HOMO: -6.80013 LUMO: -2.54154 factor:1 | -1 (0.43906) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.99429 HOMO: -6.68040 LUMO: -0.89798 factor:1 | -1 (0.57971) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.14585 HOMO: -7.01782 LUMO: -1.09662 factor:1 | -1 (0.42814) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.00253 HOMO: -6.58516 LUMO: -0.83539 factor:1 | -1 (0.57147) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.39084 HOMO: -7.46953 LUMO: 0.06259 factor:1 | -1 (0.18316) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.73896 HOMO: -6.96884 LUMO: -0.99866 factor:1 | -1 (0.83504) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.17646 HOMO: -7.29809 LUMO: -0.19320 factor:1 | -1 (2.39754) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.15624 HOMO: -6.86271 LUMO: 0.04082 factor:1 | -1 (2.41776) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.22310 HOMO: -6.36746 LUMO: -1.02587 factor:1 | -1 (2.35090) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.85310 HOMO: -7.15659 LUMO: -1.25989 factor:1 | -1 (1.72090) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.00069 HOMO: -6.69128 LUMO: -0.59865 factor:1 | -1 (1.57331) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.49799 HOMO: -7.09129 LUMO: -1.08573 factor:1 | -1 (2.07601) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.06383 HOMO: -6.64502 LUMO: -0.66396 factor:1 | -1 (2.51017) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.26209 HOMO: -6.93346 LUMO: -0.87349 factor:1 | -1 (2.31191) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.64541 HOMO: -6.77019 LUMO: -0.87349 factor:1 | -1 (0.92859) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.84234 HOMO: -6.59060 LUMO: -0.82995 factor:1 | -1 (0.73166) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.62933 HOMO: -7.17564 LUMO: -1.08846 factor:1 | -1 (0.94467) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.15507 HOMO: -7.27088 LUMO: -1.18642 factor:1 | -1 (2.41893) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.11012 HOMO: -7.06680 LUMO: -1.13199 factor:1 | -1 (2.46388) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.16884 HOMO: -7.21918 LUMO: -1.03947 factor:1 | -1 (2.40516) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.22525 HOMO: -7.26000 LUMO: -0.11973 factor:1 | -1 (2.34875) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.80357 HOMO: -6.77564 LUMO: 0.23402 factor:1 | -1 (1.77043) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.44686 HOMO: -7.07224 LUMO: -0.75648 factor:1 | -1 (2.12714) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.45350 HOMO: -7.45048 LUMO: 0.18232 factor:1 | -1 (2.12050) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.44863 HOMO: -7.48313 LUMO: 0.15238 factor:1 | -1 (2.12537) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11602 HOMO: -6.60692 LUMO: -0.50885 factor:1 | 1 (-0.54202) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.16349 HOMO: -6.62869 LUMO: -0.60954 factor:1 | -1 (0.41051) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43544 HOMO: -7.40422 LUMO: -1.28982 factor:1 | -1 (0.13856) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71498 HOMO: -6.75114 LUMO: -1.23268 factor:1 | 1 (-0.14098) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.16323 HOMO: -6.84638 LUMO: -0.73199 factor:1 | 1 (-1.58923) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.23619 HOMO: -6.79196 LUMO: -1.43676 factor:1 | 1 (-0.66219) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.09378 HOMO: -7.00965 LUMO: -1.37690 factor:1 | 1 (-1.51978) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48803 HOMO: -6.97972 LUMO: -1.58098 factor:1 | 1 (-0.91403) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72644 HOMO: -6.91169 LUMO: -1.48574 factor:1 | 1 (-0.15244) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12361 HOMO: -6.90081 LUMO: -1.30343 factor:1 | 1 (-0.54962) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08089 HOMO: -6.78652 LUMO: -1.51840 factor:1 | 1 (-0.50689) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77642 HOMO: -6.84638 LUMO: -1.15104 factor:1 | 1 (-1.20242) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.69875 HOMO: -6.61237 LUMO: -0.89798 factor:1 | 1 (-1.12476) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97888 HOMO: -7.16204 LUMO: -1.30070 factor:1 | 1 (-0.40488) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86198 HOMO: -7.32803 LUMO: 0.14694 factor:1 | 1 (-0.28798) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10993 HOMO: -6.99877 LUMO: -0.87621 factor:1 | 1 (-0.53593) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.62492 HOMO: -6.99877 LUMO: -0.97145 factor:1 | -1 (0.94908) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.58503 HOMO: -7.08040 LUMO: -1.09662 factor:1 | -1 (0.98897) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.59216 HOMO: -6.90897 LUMO: -1.14016 factor:1 | -1 (0.98184) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.56116 HOMO: -6.68312 LUMO: -0.74831 factor:1 | -1 (1.01283) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.82052 HOMO: -6.99061 LUMO: -0.86804 factor:1 | -1 (1.75347) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.81734 HOMO: -7.10761 LUMO: -1.18642 factor:1 | -1 (1.75666) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.86170 HOMO: -6.79196 LUMO: -0.71294 factor:1 | -1 (1.71230) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.93674 HOMO: -6.86271 LUMO: -0.81362 factor:1 | -1 (0.63726) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.59352 HOMO: -7.01510 LUMO: -0.99322 factor:1 | -1 (0.98048) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.36130 HOMO: -6.88720 LUMO: -0.87893 factor:1 | -1 (1.21270) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.42393 HOMO: -6.88448 LUMO: 0.22041 factor:1 | -1 (0.15007) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.69491 HOMO: -7.55932 LUMO: 1.12111 factor:1 | -1 (0.87909) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.83918 HOMO: -6.46815 LUMO: -0.86260 factor:1 | -1 (0.73482) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.40643 HOMO: -7.13755 LUMO: 0.23130 factor:1 | -1 (0.16757) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76372 HOMO: -6.78924 LUMO: 1.51023 factor:1 | 1 (-0.18972) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62790 HOMO: -6.48992 LUMO: 1.74969 factor:1 | 1 (-0.05391) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61056 HOMO: -6.78380 LUMO: 1.81500 factor:1 | 1 (-1.03656) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85146 HOMO: -6.49536 LUMO: 1.70615 factor:1 | 1 (-1.27747) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14587 HOMO: -6.38651 LUMO: 1.44492 factor:1 | 1 (-0.57187) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55570 HOMO: -6.83822 LUMO: 1.38234 factor:1 | 1 (-0.98171) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67057 HOMO: -6.01644 LUMO: 1.20274 factor:1 | 1 (-0.09657) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50716 HOMO: -6.18243 LUMO: 1.77962 factor:1 | 1 (-0.93316) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78410 HOMO: -6.81917 LUMO: -1.01771 factor:1 | 1 (-0.21010) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54224 HOMO: -6.61237 LUMO: -0.91702 factor:1 | -1 (0.03176) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90703 HOMO: -6.84094 LUMO: -0.84900 factor:1 | 1 (-1.33303) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21738 HOMO: -6.81917 LUMO: -1.01771 factor:1 | 1 (-0.64339) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92486 HOMO: -7.86953 LUMO: 1.16737 factor:1 | 1 (-0.35086) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94731 HOMO: -7.40694 LUMO: 0.11429 factor:1 | 1 (-0.37331) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11499 HOMO: -6.70489 LUMO: -0.65035 factor:1 | 1 (-0.54099) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82345 HOMO: -7.23279 LUMO: 0.33470 factor:1 | 1 (-0.24945) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.84636 HOMO: -7.17020 LUMO: 0.41361 factor:1 | -1 (2.72764) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.94146 HOMO: -6.90353 LUMO: -0.90070 factor:1 | -1 (2.63254) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.90026 HOMO: -7.39061 LUMO: 0.17687 factor:1 | -1 (2.67374) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.21929 HOMO: -7.16748 LUMO: 0.42178 factor:1 | -1 (2.35471) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.95742 HOMO: -7.36884 LUMO: -1.11295 factor:1 | -1 (1.61657) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.64387 HOMO: -7.33347 LUMO: 0.33198 factor:1 | -1 (1.93013) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.15512 HOMO: -7.31986 LUMO: -0.83539 factor:1 | -1 (1.41888) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.82082 HOMO: -7.31170 LUMO: 0.08708 factor:1 | -1 (1.75318) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.45014 HOMO: -7.36884 LUMO: 0.38096 factor:1 | -1 (1.12386) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.27504 HOMO: -6.99333 LUMO: 1.74153 factor:1 | -1 (1.29896) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.20619 HOMO: -6.94435 LUMO: 1.74969 factor:1 | -1 (1.36781) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.36110 HOMO: -7.02598 LUMO: 1.43404 factor:1 | -1 (3.21290) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.89237 HOMO: -6.41100 LUMO: 1.62996 factor:1 | -1 (2.68163) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.81852 HOMO: -6.57699 LUMO: 1.81228 factor:1 | -1 (2.75548) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.19495 HOMO: -6.86543 LUMO: 1.49935 factor:1 | -1 (1.37905) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.88217 HOMO: -6.91169 LUMO: -1.22451 factor:1 | -1 (2.69183) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.86268 HOMO: -7.09945 LUMO: -1.23812 factor:1 | -1 (2.71132) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.21385 HOMO: -7.48857 LUMO: 0.10340 factor:1 | -1 (2.36015) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.21755 HOMO: -7.21918 LUMO: -0.06803 factor:1 | -1 (2.35645) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.89038 HOMO: -6.34025 LUMO: -0.68845 factor:1 | -1 (1.68362) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.74338 HOMO: -6.82734 LUMO: -0.77825 factor:1 | -1 (1.83062) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.16628 HOMO: -6.92258 LUMO: -1.03675 factor:1 | -1 (2.40772) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.45891 HOMO: -6.42461 LUMO: -0.95240 factor:1 | -1 (2.11509) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.20552 HOMO: -6.96067 LUMO: -1.05036 factor:1 | -1 (2.36848) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.48871 HOMO: -7.23551 LUMO: 0.12245 factor:1 | -1 (2.08529) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.09090 HOMO: -6.85183 LUMO: 0.16055 factor:1 | -1 (1.48310) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.29901 HOMO: -6.46815 LUMO: -0.89253 factor:1 | -1 (1.27499) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81150 HOMO: -7.23823 LUMO: -0.06259 factor:1 | 1 (-0.23750) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84062 HOMO: -6.76475 LUMO: -0.99049 factor:1 | 1 (-0.26662) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.80803 HOMO: -7.14843 LUMO: -0.88165 factor:1 | -1 (0.76597) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.12493 HOMO: -7.15659 LUMO: 0.20681 factor:1 | -1 (0.44907) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95128 HOMO: -7.11306 LUMO: 0.14150 factor:1 | 1 (-0.37729) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.32757 HOMO: -6.67223 LUMO: -0.86260 factor:1 | -1 (0.24643) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88320 HOMO: -6.92530 LUMO: 0.30749 factor:1 | 1 (-0.30920) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.85439 HOMO: -6.50624 LUMO: -0.70477 factor:1 | -1 (0.71961) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53607 HOMO: -7.35524 LUMO: 0.75103 factor:1 | -1 (0.03793) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07107 HOMO: -7.07768 LUMO: -0.26939 factor:1 | 1 (-0.49707) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.58973 HOMO: -7.15932 LUMO: 0.42450 factor:1 | 1 (-0.01573) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.15488 HOMO: -7.46136 LUMO: 0.04626 factor:1 | -1 (2.41912) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.50844 HOMO: -7.05047 LUMO: -1.06669 factor:1 | -1 (2.06556) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.37007 HOMO: -6.66951 LUMO: -0.99322 factor:1 | -1 (2.20393) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.46000 HOMO: -7.01782 LUMO: -1.08846 factor:1 | -1 (2.11400) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.46123 HOMO: -7.03959 LUMO: -1.15376 factor:1 | -1 (2.11277) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.14550 HOMO: -6.68856 LUMO: 1.61364 factor:1 | -1 (3.42850) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.20475 HOMO: -6.53345 LUMO: 1.60275 factor:1 | -1 (1.36925) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.23715 HOMO: -6.73482 LUMO: 1.86398 factor:1 | -1 (0.33685) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.66242 HOMO: -6.87632 LUMO: 1.59731 factor:1 | -1 (0.91158) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02554 HOMO: -6.31848 LUMO: 2.12521 factor:1 | 1 (-0.45155) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93036 HOMO: -6.35114 LUMO: 1.71432 factor:1 | 1 (-0.35636) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01363 HOMO: -6.34842 LUMO: 1.92929 factor:1 | 1 (-0.43963) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.36912 HOMO: -6.14977 LUMO: 1.78235 factor:1 | -1 (0.20487) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97041 HOMO: -6.31032 LUMO: 1.51567 factor:1 | 1 (-0.39642) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.04613 HOMO: -6.25862 LUMO: 1.75241 factor:1 | -1 (0.52787) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83338 HOMO: -6.49264 LUMO: 1.66806 factor:1 | 1 (-0.25938) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.20980 HOMO: -6.28311 LUMO: 1.60003 factor:1 | -1 (0.36420) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.90343 HOMO: -7.13210 LUMO: -0.04354 factor:1 | -1 (0.67057) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11480 HOMO: -7.35252 LUMO: 0.03537 factor:1 | 1 (-0.54080) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50861 HOMO: -6.58243 LUMO: -0.48980 factor:1 | -1 (0.06539) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.05747 HOMO: -6.90081 LUMO: -0.05442 factor:1 | -1 (0.51653) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03414 HOMO: -7.22734 LUMO: 0.17143 factor:1 | 1 (-0.46014) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.59652 HOMO: -7.13210 LUMO: -0.99866 factor:1 | -1 (1.97748) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.81957 HOMO: -7.39878 LUMO: 0.13334 factor:1 | -1 (1.75443) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.91204 HOMO: -7.04503 LUMO: -0.89798 factor:1 | -1 (1.66196) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.42249 HOMO: -6.95523 LUMO: -1.07213 factor:1 | -1 (1.15150) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.47139 HOMO: -6.75114 LUMO: -1.28438 factor:1 | 1 (-1.89740) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77048 HOMO: -6.75114 LUMO: -0.11701 factor:1 | 1 (-1.19648) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.67978 HOMO: -6.83278 LUMO: -0.01633 factor:1 | 1 (-2.10578) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.41518 HOMO: -6.93890 LUMO: -0.88981 factor:1 | 1 (-1.84118) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.44032 HOMO: -7.07224 LUMO: -1.08573 factor:1 | 1 (-1.86632) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83617 HOMO: -6.99877 LUMO: -0.95240 factor:1 | 1 (-1.26217) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.52048 HOMO: -7.09129 LUMO: 0.35375 factor:1 | 1 (-1.94648) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.83312 HOMO: -7.09401 LUMO: 0.04354 factor:1 | 1 (-2.25912) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.45156 HOMO: -6.85183 LUMO: -0.68573 factor:1 | 1 (-1.87756) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43072 HOMO: -6.83006 LUMO: -0.58777 factor:1 | 1 (-0.85672) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66060 HOMO: -7.40422 LUMO: 0.17687 factor:1 | 1 (-1.08661) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.21523 HOMO: -7.15932 LUMO: 0.10340 factor:1 | 1 (-1.64123) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.21776 HOMO: -7.03414 LUMO: -0.19592 factor:1 | 1 (-1.64376) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.33275 HOMO: -6.48447 LUMO: -0.36191 factor:1 | 1 (-1.75875) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.71315 HOMO: -7.49402 LUMO: 0.11429 factor:1 | 1 (-1.13915) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.38508 HOMO: -7.01237 LUMO: -1.06397 factor:1 | 1 (-1.81108) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.18554 HOMO: -6.67223 LUMO: -1.07213 factor:1 | 1 (-1.61154) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.71883 HOMO: -7.38789 LUMO: -1.15376 factor:1 | 1 (-2.14483) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73644 HOMO: -6.42461 LUMO: -1.23812 factor:1 | 1 (-1.16244) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.47101 HOMO: -7.36884 LUMO: -1.19186 factor:1 | 1 (-1.89701) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52302 HOMO: -6.65591 LUMO: 0.07075 factor:1 | 1 (-0.94902) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.01966 HOMO: -7.39061 LUMO: -0.16871 factor:1 | 1 (-1.44566) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.40879 HOMO: -6.90353 LUMO: -0.96056 factor:1 | 1 (-0.83479) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.22023 HOMO: -7.42054 LUMO: 0.19048 factor:1 | 1 (-1.64623) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.33917 HOMO: -7.40150 LUMO: 0.35647 factor:1 | 1 (-1.76518) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.31289 HOMO: -6.56067 LUMO: -0.96056 factor:1 | 1 (-1.73889) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.99818 HOMO: -6.89809 LUMO: -0.81090 factor:1 | 1 (-2.42418) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17757 HOMO: -6.91986 LUMO: -0.84900 factor:1 | 1 (-1.60357) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.11600 HOMO: -6.61509 LUMO: -0.62042 factor:1 | -1 (0.45799) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.41188 HOMO: -6.58243 LUMO: -0.65579 factor:1 | 1 (-1.83788) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79095 HOMO: -6.52257 LUMO: -0.92519 factor:1 | 1 (-1.21695) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45731 HOMO: -6.69128 LUMO: 1.49118 factor:1 | 1 (-0.88331) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.03718 HOMO: -7.02870 LUMO: 1.67894 factor:1 | 1 (-1.46318) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.87604 HOMO: -6.88720 LUMO: 1.68711 factor:1 | 1 (-1.30204) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06280 HOMO: -5.89943 LUMO: 1.03675 factor:1 | 1 (-0.48880) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05210 HOMO: -6.40556 LUMO: 1.14560 factor:1 | 1 (-0.47810) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92799 HOMO: -6.51168 LUMO: 1.48030 factor:1 | 1 (-0.35399) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97039 HOMO: -6.64502 LUMO: 1.91568 factor:1 | 1 (-0.39639) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86225 HOMO: -6.47903 LUMO: 1.91296 factor:1 | 1 (-0.28825) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.40268 HOMO: -6.34297 LUMO: 1.91840 factor:1 | -1 (1.17131) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10530 HOMO: -6.89809 LUMO: 1.82861 factor:1 | 1 (-0.53130) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.14403 HOMO: -6.10079 LUMO: 1.62996 factor:1 | -1 (0.42997) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95814 HOMO: -7.16476 LUMO: -0.92247 factor:1 | 1 (-0.38414) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16255 HOMO: -7.10489 LUMO: -0.95784 factor:1 | 1 (-0.58856) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23044 HOMO: -6.76475 LUMO: -0.99866 factor:1 | 1 (-1.65644) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.25030 HOMO: -6.81373 LUMO: -1.05036 factor:1 | 1 (-1.67630) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.14976 HOMO: -6.90081 LUMO: -1.03947 factor:1 | 1 (-1.57576) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.61526 HOMO: -7.06952 LUMO: -0.91702 factor:1 | 1 (-2.04126) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.03843 HOMO: -6.73482 LUMO: -0.94151 factor:1 | 1 (-1.46444) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29896 HOMO: -6.99605 LUMO: -1.04764 factor:1 | 1 (-0.72497) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.17642 HOMO: -7.03686 LUMO: -0.93335 factor:1 | 1 (-1.60242) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.32938 HOMO: -6.81101 LUMO: -0.95240 factor:1 | 1 (-1.75538) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.27768 HOMO: -6.83822 LUMO: -0.65307 factor:1 | 1 (-1.70368) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93008 HOMO: -7.05319 LUMO: -0.81634 factor:1 | 1 (-1.35608) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79699 HOMO: -7.57565 LUMO: 0.19048 factor:1 | 1 (-1.22299) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01398 HOMO: -6.56067 LUMO: -0.50613 factor:1 | 1 (-0.43998) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92029 HOMO: -6.74298 LUMO: -0.70477 factor:1 | 1 (-0.34629) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69046 HOMO: -7.02054 LUMO: 0.03537 factor:1 | 1 (-0.11646) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98720 HOMO: -7.33347 LUMO: -0.17960 factor:1 | 1 (-0.41320) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.70272 HOMO: -6.98244 LUMO: -0.88165 factor:1 | 1 (-2.12872) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.76185 HOMO: -7.14843 LUMO: -1.19730 factor:1 | 1 (-2.18785) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.43191 HOMO: -7.17564 LUMO: -1.21907 factor:1 | 1 (-1.85791) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.20538 HOMO: -6.74026 LUMO: -0.86532 factor:1 | 1 (-1.63138) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.34686 HOMO: -6.82462 LUMO: -1.24084 factor:1 | 1 (-0.77286) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51573 HOMO: -6.78924 LUMO: -0.70477 factor:1 | 1 (-0.94173) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86036 HOMO: -7.41238 LUMO: 0.05987 factor:1 | 1 (-1.28636) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73789 HOMO: -6.75931 LUMO: 0.02721 factor:1 | 1 (-0.16389) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.25422 HOMO: -6.28583 LUMO: -0.93063 factor:1 | 1 (-1.68022) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53530 HOMO: -6.69128 LUMO: -0.83539 factor:1 | 1 (-0.96130) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41562 HOMO: -7.22190 LUMO: 0.01361 factor:1 | 1 (-0.84162) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92640 HOMO: -6.95251 LUMO: -1.09934 factor:1 | 1 (-1.35241) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48507 HOMO: -6.75387 LUMO: -0.90614 factor:1 | -1 (0.08893) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13448 HOMO: -7.48585 LUMO: 0.05987 factor:1 | -1 (0.43952) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.81390 HOMO: -6.92802 LUMO: -0.66940 factor:1 | -1 (0.76010) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.24978 HOMO: -7.29537 LUMO: -0.14150 factor:1 | -1 (0.32422) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86652 HOMO: -6.57155 LUMO: -0.86804 factor:1 | 1 (-0.29252) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.07723 HOMO: -6.87632 LUMO: -0.77825 factor:1 | -1 (0.49677) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.90278 HOMO: -6.45998 LUMO: -0.31565 factor:1 | -1 (0.67122) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65664 HOMO: -7.51306 LUMO: 0.05714 factor:1 | 1 (-0.08264) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.41435 HOMO: -6.86271 LUMO: -0.00816 factor:1 | -1 (0.15965) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19630 HOMO: -6.43277 LUMO: -1.07485 factor:1 | -1 (0.37769) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97254 HOMO: -6.78108 LUMO: -0.81362 factor:1 | 1 (-0.39854) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.40290 HOMO: -6.88448 LUMO: 1.21907 factor:1 | 1 (-1.82890) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.95838 HOMO: -6.97700 LUMO: 1.44765 factor:1 | 1 (-1.38438) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.18989 HOMO: -6.89537 LUMO: 2.12249 factor:1 | 1 (-1.61589) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.96585 HOMO: -6.28311 LUMO: 1.45037 factor:1 | 1 (-2.39185) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.74802 HOMO: -6.55522 LUMO: 1.39867 factor:1 | 1 (-3.17402) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92613 HOMO: -6.46815 LUMO: 1.50207 factor:1 | 1 (-1.35213) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96016 HOMO: -6.43549 LUMO: 2.17419 factor:1 | 1 (-0.38616) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73700 HOMO: -6.99333 LUMO: 1.87214 factor:1 | 1 (-0.16300) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83634 HOMO: -6.65591 LUMO: 1.37962 factor:1 | 1 (-0.26234) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78837 HOMO: -6.82734 LUMO: 1.55649 factor:1 | 1 (-0.21437) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79153 HOMO: -6.71849 LUMO: 1.36057 factor:1 | 1 (-0.21753) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54023 HOMO: -6.79468 LUMO: 1.82044 factor:1 | -1 (0.03377) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62935 HOMO: -6.61237 LUMO: 1.15104 factor:1 | 1 (-0.05535) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43601 HOMO: -6.62053 LUMO: 2.33474 factor:1 | -1 (0.13799) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72102 HOMO: -6.55794 LUMO: 1.65717 factor:1 | 1 (-0.14702) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73577 HOMO: -6.85999 LUMO: 2.03813 factor:1 | 1 (-0.16177) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57509 HOMO: -6.45726 LUMO: 1.28438 factor:1 | 1 (-0.00109) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71196 HOMO: -6.23685 LUMO: 1.93201 factor:1 | 1 (-0.13796) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91958 HOMO: -7.06680 LUMO: 1.86942 factor:1 | 1 (-0.34558) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10465 HOMO: -6.89537 LUMO: 2.17147 factor:1 | 1 (-0.53065) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52733 HOMO: -6.80013 LUMO: 1.78779 factor:1 | -1 (0.04667) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52611 HOMO: -6.45726 LUMO: 1.58370 factor:1 | -1 (0.04789) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.14406 HOMO: -6.52529 LUMO: 1.71976 factor:1 | -1 (0.42994) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73914 HOMO: -7.22462 LUMO: -1.18642 factor:1 | 1 (-0.16515) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00709 HOMO: -7.18381 LUMO: -0.78641 factor:1 | 1 (-1.43309) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28696 HOMO: -6.93346 LUMO: 1.65717 factor:1 | 1 (-0.71297) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.85073 HOMO: -6.41644 LUMO: 1.78235 factor:1 | 1 (-1.27673) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00728 HOMO: -6.59876 LUMO: 1.83677 factor:1 | 1 (-1.43328) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.49917 HOMO: -6.35658 LUMO: 1.59731 factor:1 | -1 (0.07483) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80432 HOMO: -6.60692 LUMO: 1.66534 factor:1 | 1 (-0.23032) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26520 HOMO: -6.83006 LUMO: 2.11705 factor:1 | -1 (0.30879) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.00196 HOMO: -6.89264 LUMO: 1.30070 factor:1 | -1 (0.57204) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64812 HOMO: -6.90081 LUMO: 2.05174 factor:1 | 1 (-0.07412) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.30611 HOMO: -6.74842 LUMO: 1.96194 factor:1 | -1 (1.26789) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.05797 HOMO: -6.58516 LUMO: 1.30887 factor:1 | -1 (1.51603) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.79233 HOMO: -7.00965 LUMO: 2.08167 factor:1 | -1 (1.78167) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29478 HOMO: -6.86815 LUMO: 2.29664 factor:1 | -1 (0.27922) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.09309 HOMO: -6.39740 LUMO: 2.02725 factor:1 | -1 (0.48091) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66769 HOMO: -5.95929 LUMO: 1.62724 factor:1 | 1 (-0.09369) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.87078 HOMO: -6.71849 LUMO: 1.34696 factor:1 | -1 (0.70322) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.11298 HOMO: -7.26816 LUMO: 1.74153 factor:1 | -1 (0.46102) | 1 | 1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.52541 HOMO: -6.90897 LUMO: 1.71432 factor:1 | -1 (1.04859) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.28926 HOMO: -6.70489 LUMO: 1.91568 factor:1 | -1 (0.28474) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89565 HOMO: -6.83278 LUMO: 1.61908 factor:1 | -1 (0.67835) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.36167 HOMO: -7.17292 LUMO: 1.95378 factor:1 | -1 (0.21233) | 1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.88623 HOMO: -6.53345 LUMO: 1.74153 factor:1 | -1 (0.68777) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54102 HOMO: -6.53073 LUMO: 1.51023 factor:1 | -1 (0.03298) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38877 HOMO: -6.93346 LUMO: 2.22861 factor:1 | -1 (0.18523) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.04780 HOMO: -6.47903 LUMO: 2.05446 factor:1 | -1 (2.52620) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.89702 HOMO: -6.88992 LUMO: 1.57010 factor:1 | -1 (2.67697) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.47355 HOMO: -6.07358 LUMO: 1.95922 factor:1 | -1 (2.10045) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.02722 HOMO: -6.75114 LUMO: 2.18780 factor:1 | -1 (1.54678) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.55641 HOMO: -6.96339 LUMO: 1.70071 factor:1 | -1 (2.01759) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.96836 HOMO: -7.14843 LUMO: 1.82588 factor:1 | -1 (1.60564) | 1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.70869 HOMO: -6.96339 LUMO: 2.29392 factor:1 | -1 (1.86531) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.77152 HOMO: -6.81645 LUMO: 2.39732 factor:1 | -1 (1.80248) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.81582 HOMO: -6.48447 LUMO: 1.24084 factor:1 | -1 (1.75818) | -1 | -1 |
| G: -5684.20830 HOMO: -7.55660 LUMO: -2.00004 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.28326 HOMO: -7.14843 LUMO: 2.01092 factor:1 | -1 (2.29074) | 1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.80864 HOMO: -7.20013 LUMO: -0.34286 factor:1 | -1 (2.76536) | 1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.00598 HOMO: -6.97700 LUMO: -0.15238 factor:1 | -1 (2.56802) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.90709 HOMO: -7.07768 LUMO: -0.26123 factor:1 | -1 (2.66691) | 1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.03324 HOMO: -6.99333 LUMO: -0.41361 factor:1 | -1 (2.54075) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.08799 HOMO: -6.84638 LUMO: -0.40273 factor:1 | -1 (2.48601) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.12802 HOMO: -6.83822 LUMO: -0.26939 factor:1 | -1 (2.44598) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.63887 HOMO: -6.75931 LUMO: -0.93879 factor:1 | -1 (2.93513) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.72537 HOMO: -6.79468 LUMO: -0.39729 factor:1 | -1 (2.84862) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.88881 HOMO: -6.93890 LUMO: 0.43266 factor:1 | -1 (2.68519) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.74557 HOMO: -7.08040 LUMO: -0.85716 factor:1 | -1 (2.82843) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.24078 HOMO: -6.70216 LUMO: -1.41499 factor:1 | -1 (1.33322) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82704 HOMO: -6.63686 LUMO: -0.52790 factor:1 | 1 (-0.25304) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56140 HOMO: -6.75114 LUMO: -0.13334 factor:1 | -1 (0.01260) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74431 HOMO: -6.94435 LUMO: -0.24490 factor:1 | 1 (-0.17032) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15674 HOMO: -6.74298 LUMO: -0.84627 factor:1 | -1 (0.41726) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.14308 HOMO: -7.15932 LUMO: 0.22041 factor:1 | -1 (0.43092) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72576 HOMO: -6.90081 LUMO: -1.16737 factor:1 | 1 (-0.15176) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13024 HOMO: -7.04775 LUMO: -0.84355 factor:1 | -1 (0.44376) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89395 HOMO: -7.17020 LUMO: -1.31159 factor:1 | 1 (-0.31995) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55550 HOMO: -7.14571 LUMO: -0.46259 factor:1 | -1 (0.01850) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.88261 HOMO: -7.45048 LUMO: -0.91158 factor:1 | -1 (0.69139) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98744 HOMO: -6.87360 LUMO: -0.82995 factor:1 | 1 (-1.41344) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05469 HOMO: -7.43415 LUMO: -0.65307 factor:1 | 1 (-0.48069) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61667 HOMO: -7.47225 LUMO: -0.77280 factor:1 | 1 (-0.04267) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44185 HOMO: -6.86271 LUMO: -0.83811 factor:1 | 1 (-0.86785) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.90290 HOMO: -7.53483 LUMO: -0.66124 factor:1 | 1 (-0.32890) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68064 HOMO: -7.45864 LUMO: -1.08301 factor:1 | 1 (-0.10664) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.62605 HOMO: -7.24639 LUMO: -1.19186 factor:1 | 1 (-1.05205) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.83695 HOMO: -7.54844 LUMO: -0.96873 factor:1 | -1 (0.73705) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.56242 HOMO: -7.12666 LUMO: -0.01633 factor:1 | -1 (1.01158) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94568 HOMO: -6.77291 LUMO: -0.70477 factor:1 | 1 (-0.37168) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69163 HOMO: -6.76475 LUMO: -1.15921 factor:1 | 1 (-0.11763) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.97616 HOMO: -5.37697 LUMO: -0.56600 factor:1 | -1 (0.59783) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.16528 HOMO: -6.62053 LUMO: -1.75513 factor:1 | -1 (0.40872) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.10425 HOMO: -6.60420 LUMO: -1.74697 factor:1 | -1 (0.46975) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.27950 HOMO: -6.84366 LUMO: -0.94968 factor:1 | -1 (1.29450) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.49689 HOMO: -6.96884 LUMO: -2.11977 factor:1 | -1 (1.07711) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.39798 HOMO: -6.80829 LUMO: 0.56055 factor:1 | -1 (1.17602) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.27603 HOMO: -7.02326 LUMO: 0.11429 factor:1 | -1 (0.29796) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.46133 HOMO: -7.40966 LUMO: 0.18232 factor:1 | -1 (1.11267) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.22203 HOMO: -6.34570 LUMO: 0.41089 factor:1 | -1 (1.35197) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.90757 HOMO: -6.78924 LUMO: 0.49525 factor:1 | -1 (1.66643) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.00401 HOMO: -6.87632 LUMO: 0.44082 factor:1 | -1 (1.56999) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.61957 HOMO: -6.69944 LUMO: 1.20546 factor:1 | -1 (1.95443) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29808 HOMO: -6.83006 LUMO: 1.28982 factor:1 | -1 (0.27592) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.32613 HOMO: -7.78246 LUMO: 0.20681 factor:1 | -1 (0.24787) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83901 HOMO: -6.55794 LUMO: -1.65173 factor:1 | 1 (-0.26501) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43492 HOMO: -6.77564 LUMO: -1.14560 factor:1 | -1 (0.13908) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92922 HOMO: -7.46680 LUMO: -1.18097 factor:1 | 1 (-0.35522) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15233 HOMO: -6.88176 LUMO: -1.24900 factor:1 | -1 (0.42167) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.46871 HOMO: -7.28177 LUMO: -0.42178 factor:1 | -1 (2.10529) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.39135 HOMO: -7.71715 LUMO: 0.19592 factor:1 | -1 (2.18265) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.66398 HOMO: -7.02326 LUMO: -1.40683 factor:1 | -1 (1.91002) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.55568 HOMO: -7.27088 LUMO: -1.07485 factor:1 | -1 (3.01831) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.39285 HOMO: -7.17020 LUMO: -0.49525 factor:1 | -1 (3.18115) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.86633 HOMO: -7.15932 LUMO: 0.02721 factor:1 | -1 (2.70767) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.64156 HOMO: -7.00693 LUMO: -0.83267 factor:1 | -1 (2.93244) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.21841 HOMO: -6.86543 LUMO: -0.10340 factor:1 | -1 (1.35559) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.56833 HOMO: -7.11850 LUMO: -0.08980 factor:1 | -1 (2.00567) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.22538 HOMO: -6.87087 LUMO: -0.88981 factor:1 | -1 (1.34862) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.45176 HOMO: -7.08857 LUMO: -1.27077 factor:1 | -1 (2.12224) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.31952 HOMO: -6.79468 LUMO: -0.81906 factor:1 | -1 (0.25448) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47683 HOMO: -6.86815 LUMO: -0.89798 factor:1 | -1 (0.09717) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.20643 HOMO: -6.78652 LUMO: -2.00548 factor:1 | -1 (0.36757) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15464 HOMO: -6.75114 LUMO: -0.08436 factor:1 | -1 (0.41935) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63258 HOMO: -6.55794 LUMO: 0.52790 factor:1 | 1 (-0.05859) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.09451 HOMO: -7.17836 LUMO: 0.28300 factor:1 | -1 (0.47949) | 1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.82577 HOMO: -7.35796 LUMO: -0.77552 factor:1 | -1 (0.74823) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.44623 HOMO: -7.23551 LUMO: -1.17553 factor:1 | -1 (2.12777) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.46484 HOMO: -7.07496 LUMO: -1.14288 factor:1 | -1 (2.10915) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.66205 HOMO: -6.70489 LUMO: -0.83539 factor:1 | -1 (1.91195) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.67543 HOMO: -6.59604 LUMO: -0.89798 factor:1 | -1 (1.89857) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.66074 HOMO: -6.94162 LUMO: -1.22451 factor:1 | -1 (1.91326) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.42176 HOMO: -6.68040 LUMO: 0.22041 factor:1 | -1 (1.15224) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.43724 HOMO: -6.88176 LUMO: 0.11157 factor:1 | -1 (1.13676) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.58500 HOMO: -6.91713 LUMO: 1.27621 factor:1 | -1 (0.98900) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54042 HOMO: -6.77836 LUMO: 1.01226 factor:1 | -1 (0.03358) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.51278 HOMO: -7.14571 LUMO: 1.48574 factor:1 | -1 (1.06122) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.62214 HOMO: -6.96884 LUMO: 1.48574 factor:1 | -1 (0.95185) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.08124 HOMO: -7.24367 LUMO: 1.28438 factor:1 | -1 (1.49276) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.46339 HOMO: -7.10489 LUMO: 1.29526 factor:1 | -1 (1.11061) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.48266 HOMO: -7.07224 LUMO: 1.29254 factor:1 | -1 (1.09134) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.94224 HOMO: -7.12938 LUMO: 0.49253 factor:1 | 1 (-1.36824) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29023 HOMO: -7.33619 LUMO: 1.45581 factor:1 | 1 (-0.71623) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.37535 HOMO: -6.87904 LUMO: -0.14422 factor:1 | 1 (-0.80135) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62328 HOMO: -6.81917 LUMO: 0.50341 factor:1 | 1 (-0.04928) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.40983 HOMO: -7.27905 LUMO: 0.13606 factor:1 | -1 (0.16417) | 1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60369 HOMO: -6.87904 LUMO: -0.09796 factor:1 | 1 (-0.02969) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77712 HOMO: -7.33891 LUMO: 0.03810 factor:1 | 1 (-1.20312) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.04280 HOMO: -6.98516 LUMO: 0.98233 factor:1 | 1 (-0.46880) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81093 HOMO: -6.94162 LUMO: 0.86804 factor:1 | 1 (-0.23693) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06272 HOMO: -7.37701 LUMO: 0.05442 factor:1 | 1 (-0.48872) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81106 HOMO: -7.04775 LUMO: 0.43266 factor:1 | 1 (-0.23707) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.77075 HOMO: -7.47497 LUMO: 0.31837 factor:1 | -1 (1.80324) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.30794 HOMO: -6.62053 LUMO: 0.13061 factor:1 | -1 (2.26606) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.56825 HOMO: -6.44366 LUMO: -0.04354 factor:1 | -1 (2.00575) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.85982 HOMO: -6.40284 LUMO: 0.68301 factor:1 | -1 (1.71418) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.53421 HOMO: -6.73754 LUMO: 0.36735 factor:1 | -1 (2.03979) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.29623 HOMO: -6.85455 LUMO: 0.23946 factor:1 | -1 (1.27777) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77112 HOMO: -6.93346 LUMO: 0.24762 factor:1 | 1 (-0.19712) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51313 HOMO: -6.85455 LUMO: 0.17687 factor:1 | -1 (0.06087) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26588 HOMO: -6.62325 LUMO: 0.69933 factor:1 | -1 (0.30811) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57808 HOMO: -6.43005 LUMO: 0.50069 factor:1 | 1 (-0.00408) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61097 HOMO: -6.56883 LUMO: 0.22858 factor:1 | 1 (-1.03697) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.33306 HOMO: -6.78380 LUMO: 0.54967 factor:1 | 1 (-0.75906) | -1 | -1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50414 HOMO: -7.35524 LUMO: 0.00272 factor:1 | 1 (-0.93014) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79958 HOMO: -7.27360 LUMO: 0.08436 factor:1 | 1 (-0.22558) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53302 HOMO: -7.44504 LUMO: -0.96056 factor:1 | -1 (0.04098) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09153 HOMO: -7.27360 LUMO: 0.29933 factor:1 | 1 (-0.51753) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.68637 HOMO: -7.09129 LUMO: 0.41089 factor:1 | 1 (-1.11237) | 1 | 1 |
| G: -5684.20830 HOMO: -8.61512 LUMO: -2.99325 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00429 HOMO: -6.93618 LUMO: 0.36463 factor:1 | 1 (-0.43029) | -1 | -1 |
| G: -5684.20830 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63620 HOMO: -7.65728 LUMO: 0.20136 factor:1 | 1 (-0.06221) | 1 | 1 |
| G: -5684.20830 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67797 HOMO: -6.90353 LUMO: -0.92791 factor:1 | 1 (-0.10397) | -1 | -1 |
| G: -5684.20830 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.55553 HOMO: -6.82462 LUMO: -1.18370 factor:1 | -1 (1.01847) | -1 | -1 |
| G: -5684.20830 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.69483 HOMO: -7.09129 LUMO: -0.13334 factor:1 | -1 (0.87917) | 1 | 1 |
| G: -5684.20830 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75626 HOMO: -7.40966 LUMO: -1.06941 factor:1 | 1 (-0.18226) | 1 | 1 |
| G: -5684.20830 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.23081 HOMO: -7.24367 LUMO: -1.00954 factor:1 | -1 (0.34319) | 1 | 1 |
| G: -5684.20830 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52047 HOMO: -7.51851 LUMO: 0.09796 factor:1 | -1 (0.05352) | 1 | 1 |
| G: -5684.20830 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.85254 HOMO: -7.48857 LUMO: -0.07619 factor:1 | -1 (0.72146) | 1 | 1 |
| G: -5684.20830 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.41604 HOMO: -6.53345 LUMO: 1.09390 factor:1 | -1 (0.15796) | -1 | -1 |
| G: -5684.20830 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62366 HOMO: -7.21918 LUMO: 0.08436 factor:1 | 1 (-0.04966) | 1 | 1 |
| G: -5684.20830 HOMO: -7.26000 LUMO: -3.02863 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.49686 HOMO: -7.38789 LUMO: 1.02587 factor:1 | 1 (-1.92287) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.00011 HOMO: -6.83550 LUMO: -0.67484 factor:1 | 1 (-2.42611) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.03411 HOMO: -7.04231 LUMO: 0.54151 factor:1 | 1 (-1.46011) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.14497 HOMO: -6.79740 LUMO: 1.91296 factor:1 | 1 (-1.57097) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.04491 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-1.47091) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.08097 HOMO: -6.62597 LUMO: -0.44082 factor:1 | 1 (-1.50697) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08900 HOMO: -6.45182 LUMO: -0.20409 factor:1 | 1 (-0.51500) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65938 HOMO: -6.51168 LUMO: -0.23130 factor:1 | 1 (-1.08538) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81286 HOMO: -7.14027 LUMO: 0.49797 factor:1 | 1 (-0.23886) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61927 HOMO: -7.55660 LUMO: 0.24762 factor:1 | 1 (-1.04527) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73807 HOMO: -6.88992 LUMO: -0.64763 factor:1 | 1 (-1.16408) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72989 HOMO: -6.72665 LUMO: -0.45987 factor:1 | 1 (-0.15589) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83070 HOMO: -6.72121 LUMO: -0.58232 factor:1 | 1 (-1.25670) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.43545 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-1.86145) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57894 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-1.00494) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.79658 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-1.22258) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96448 HOMO: -6.73210 LUMO: -0.51430 factor:1 | 1 (-0.39048) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.09326 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-1.51927) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44599 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-0.87199) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78042 HOMO: -6.79740 LUMO: -0.55511 factor:1 | 1 (-0.20643) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.12829 HOMO: -6.79740 LUMO: -0.67756 factor:1 | 1 (-1.55429) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.76120 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-2.18720) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55290 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-0.97890) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.47793 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-1.90393) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86855 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-1.29455) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77794 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-1.20394) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.99169 HOMO: -6.59332 LUMO: -0.27211 factor:1 | 1 (-0.41769) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.42213 HOMO: -6.57427 LUMO: -0.16871 factor:1 | -1 (0.15187) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02821 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-0.45421) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.00966 HOMO: -6.72121 LUMO: 2.00004 factor:1 | -1 (0.56434) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.20022 HOMO: -6.61509 LUMO: 1.55921 factor:1 | -1 (0.37378) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07390 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-0.49990) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50409 HOMO: -6.66135 LUMO: 2.02181 factor:1 | -1 (0.06991) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.40203 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-1.82803) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99653 HOMO: -6.66679 LUMO: 1.98371 factor:1 | 1 (-1.42253) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39537 HOMO: -6.67495 LUMO: 2.04085 factor:1 | 1 (-0.82138) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67173 HOMO: -6.89809 LUMO: 1.95106 factor:1 | 1 (-1.09773) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06103 HOMO: -6.50352 LUMO: 1.88847 factor:1 | 1 (-0.48703) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57018 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-0.99618) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.67440 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-1.10040) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67226 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-0.09826) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82679 HOMO: -6.65591 LUMO: 2.20684 factor:1 | 1 (-0.25279) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10443 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-0.53043) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79838 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-0.22439) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88690 HOMO: -6.53617 LUMO: 1.75241 factor:1 | 1 (-0.31290) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.00568 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-0.43168) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.75693 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-1.18293) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11483 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-0.54083) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83982 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-1.26582) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.42143 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-1.84744) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.51632 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-1.94232) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.82816 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-2.25416) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.03492 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-1.46092) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.78186 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-1.20786) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.30853 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-1.73454) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.89717 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-2.32317) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.66091 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-3.08691) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.88210 HOMO: -6.90897 LUMO: 1.91296 factor:1 | 1 (-2.30810) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11951.03429 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-2.46029) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.33400 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-1.76001) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.94169 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-2.36769) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.54644 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-1.97244) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.65540 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-2.08140) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.05626 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-1.48226) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.34133 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-0.76733) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.24089 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-1.66689) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.19357 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-1.61957) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.40367 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-0.82968) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.49227 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-0.91828) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38996 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-0.81596) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72777 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-0.15377) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84179 HOMO: -6.75387 LUMO: 1.72248 factor:1 | 1 (-0.26779) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76668 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-0.19268) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87964 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-0.30564) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.06031 HOMO: -6.80557 LUMO: 2.02725 factor:1 | -1 (1.51369) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92214 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-0.34814) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70426 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-0.13026) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84739 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-0.27339) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97930 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-1.40530) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.38843 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-1.81443) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93237 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-0.35837) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66214 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-0.08814) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91001 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-0.33601) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.37686 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-1.80286) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.02499 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-1.45099) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.74726 HOMO: -6.69128 LUMO: 1.70888 factor:1 | -1 (0.82674) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61451 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-1.04051) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77340 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-1.19940) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88500 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-0.31100) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88960 HOMO: -6.64230 LUMO: 2.16058 factor:1 | 1 (-0.31560) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53539 HOMO: -6.58788 LUMO: 2.10616 factor:1 | -1 (0.03861) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89205 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-0.31805) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07243 HOMO: -6.31304 LUMO: 2.31841 factor:1 | 1 (-0.49843) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74148 HOMO: -6.94979 LUMO: 2.07895 factor:1 | 1 (-0.16749) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74880 HOMO: -6.88992 LUMO: 2.28031 factor:1 | 1 (-0.17481) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74290 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-0.16890) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51348 HOMO: -6.52529 LUMO: 1.70071 factor:1 | -1 (0.06052) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55258 HOMO: -6.58788 LUMO: 1.57282 factor:1 | -1 (0.02142) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19220 HOMO: -6.55250 LUMO: 1.95378 factor:1 | -1 (0.38180) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67245 HOMO: -6.24773 LUMO: 1.77962 factor:1 | 1 (-0.09845) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.05596 HOMO: -6.31304 LUMO: 2.18507 factor:1 | -1 (1.51804) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.77784 HOMO: -6.18243 LUMO: 2.01636 factor:1 | -1 (2.79616) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.05520 HOMO: -6.99877 LUMO: 2.14970 factor:1 | -1 (2.51879) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.07399 HOMO: -6.72665 LUMO: 2.07079 factor:1 | -1 (0.50001) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67310 HOMO: -6.36202 LUMO: 2.17419 factor:1 | 1 (-0.09910) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.34240 HOMO: -6.78652 LUMO: 2.05718 factor:1 | -1 (0.23160) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94445 HOMO: -6.87360 LUMO: 2.34290 factor:1 | 1 (-0.37046) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.27818 HOMO: -6.62053 LUMO: 1.89391 factor:1 | -1 (0.29581) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.77846 HOMO: -6.58788 LUMO: 1.83133 factor:1 | -1 (1.79554) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.80594 HOMO: -7.08584 LUMO: 1.91568 factor:1 | -1 (1.76806) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.78270 HOMO: -6.56883 LUMO: 1.81228 factor:1 | -1 (1.79130) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47762 HOMO: -6.66135 LUMO: 1.92384 factor:1 | -1 (0.09638) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72649 HOMO: -6.64502 LUMO: 2.15786 factor:1 | 1 (-0.15249) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11496 HOMO: -6.71305 LUMO: 1.91840 factor:1 | 1 (-0.54096) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08585 HOMO: -6.44094 LUMO: 1.74425 factor:1 | 1 (-0.51185) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.43416 HOMO: -6.51985 LUMO: 1.84221 factor:1 | -1 (0.13984) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77330 HOMO: -6.63414 LUMO: -0.24762 factor:1 | 1 (-0.19930) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77370 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-0.19970) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.10860 HOMO: -7.19741 LUMO: 0.58232 factor:1 | -1 (0.46540) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.92849 HOMO: -6.77019 LUMO: -0.56872 factor:1 | -1 (0.64551) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97792 HOMO: -7.46136 LUMO: 0.28844 factor:1 | 1 (-0.40393) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.34774 HOMO: -6.60420 LUMO: -0.54151 factor:1 | -1 (0.22626) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26809 HOMO: -6.53890 LUMO: -0.46531 factor:1 | -1 (0.30591) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.42036 HOMO: -6.81645 LUMO: -0.57144 factor:1 | -1 (0.15364) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56676 HOMO: -7.48041 LUMO: 0.28572 factor:1 | -1 (0.00724) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71599 HOMO: -6.75659 LUMO: -0.45715 factor:1 | 1 (-0.14199) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21904 HOMO: -6.66135 LUMO: -0.41906 factor:1 | 1 (-0.64505) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87172 HOMO: -6.55794 LUMO: -0.27483 factor:1 | 1 (-0.29772) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68437 HOMO: -7.07496 LUMO: -0.63403 factor:1 | 1 (-0.11037) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68801 HOMO: -7.12394 LUMO: 0.53334 factor:1 | 1 (-0.11402) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65465 HOMO: -6.53617 LUMO: -0.25579 factor:1 | 1 (-0.08065) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.40844 HOMO: -6.50896 LUMO: -0.25034 factor:1 | -1 (0.16555) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54355 HOMO: -7.17564 LUMO: -0.68573 factor:1 | -1 (0.03045) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.86311 HOMO: -6.53617 LUMO: -0.30749 factor:1 | -1 (1.71089) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.99472 HOMO: -6.55522 LUMO: -0.30749 factor:1 | -1 (0.57928) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.35900 HOMO: -7.05591 LUMO: -0.71022 factor:1 | -1 (0.21500) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76301 HOMO: -7.17564 LUMO: -0.69933 factor:1 | 1 (-0.18901) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.68310 HOMO: -6.78380 LUMO: -0.67756 factor:1 | -1 (0.89090) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.82049 HOMO: -6.62325 LUMO: 2.02725 factor:1 | -1 (0.75351) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.88174 HOMO: -6.63414 LUMO: 1.91296 factor:1 | -1 (0.69226) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93376 HOMO: -6.83278 LUMO: 1.65717 factor:1 | 1 (-0.35976) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89467 HOMO: -6.66407 LUMO: 1.95650 factor:1 | -1 (0.67933) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.23334 HOMO: -6.61237 LUMO: 2.11432 factor:1 | -1 (0.34066) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.28692 HOMO: -6.62053 LUMO: 2.09256 factor:1 | -1 (0.28708) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11943.79832 HOMO: -6.78652 LUMO: 2.13609 factor:1 | -1 (4.77568) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.24730 HOMO: -6.94707 LUMO: 1.81772 factor:1 | -1 (0.32670) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.83600 HOMO: -6.85183 LUMO: 2.12793 factor:1 | -1 (0.73800) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.36905 HOMO: -6.81101 LUMO: 1.83949 factor:1 | -1 (1.20495) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.40228 HOMO: -6.98788 LUMO: 2.16058 factor:1 | -1 (1.17172) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.00302 HOMO: -6.62869 LUMO: 2.00820 factor:1 | -1 (0.57098) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.48043 HOMO: -6.34025 LUMO: 2.25855 factor:1 | -1 (1.09357) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87264 HOMO: -6.01372 LUMO: 2.01636 factor:1 | 1 (-0.29864) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91624 HOMO: -6.89264 LUMO: 2.27487 factor:1 | 1 (-0.34224) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.28583 HOMO: -6.53073 LUMO: 2.20684 factor:1 | -1 (0.28817) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82848 HOMO: -6.83278 LUMO: 1.53744 factor:1 | 1 (-0.25448) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.10594 HOMO: -6.41917 LUMO: 1.82316 factor:1 | -1 (0.46806) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.33876 HOMO: -6.56339 LUMO: 1.63813 factor:1 | -1 (0.23524) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94279 HOMO: -6.88992 LUMO: 1.65173 factor:1 | 1 (-0.36880) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.33190 HOMO: -6.63141 LUMO: 1.92112 factor:1 | -1 (0.24210) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.83145 HOMO: -6.83822 LUMO: 1.88847 factor:1 | -1 (0.74254) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44496 HOMO: -6.84638 LUMO: 1.90480 factor:1 | -1 (0.12904) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.98510 HOMO: -6.82462 LUMO: 1.70888 factor:1 | -1 (1.58890) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.85051 HOMO: -6.82734 LUMO: 2.12521 factor:1 | -1 (1.72349) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.85323 HOMO: -6.94435 LUMO: 1.87214 factor:1 | -1 (1.72077) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.30509 HOMO: -6.98516 LUMO: 2.51433 factor:1 | -1 (2.26891) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.40180 HOMO: -6.74026 LUMO: 2.15514 factor:1 | -1 (2.17220) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62350 HOMO: -6.93618 LUMO: 2.54426 factor:1 | 1 (-0.04950) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83645 HOMO: -6.28583 LUMO: 2.53610 factor:1 | 1 (-0.26245) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69697 HOMO: -6.56883 LUMO: 1.94834 factor:1 | 1 (-0.12297) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77784 HOMO: -7.08584 LUMO: 1.99187 factor:1 | 1 (-0.20384) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13992 HOMO: -6.19059 LUMO: 1.99732 factor:1 | -1 (0.43408) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.70334 HOMO: -6.78108 LUMO: 2.03813 factor:1 | -1 (0.87066) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69131 HOMO: -6.82189 LUMO: 1.77418 factor:1 | 1 (-0.11731) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96669 HOMO: -6.45454 LUMO: 1.78779 factor:1 | 1 (-0.39269) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.34050 HOMO: -6.84366 LUMO: 1.77690 factor:1 | -1 (0.23350) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.87360 HOMO: -6.74026 LUMO: 1.67622 factor:1 | -1 (0.70039) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.70868 HOMO: -6.76475 LUMO: 2.40277 factor:1 | -1 (0.86532) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.59240 HOMO: -6.65863 LUMO: 1.86670 factor:1 | -1 (0.98160) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94566 HOMO: -6.50080 LUMO: 1.93201 factor:1 | -1 (0.62834) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.77918 HOMO: -6.34842 LUMO: 1.70888 factor:1 | -1 (0.79482) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.13543 HOMO: -6.60692 LUMO: 2.20140 factor:1 | -1 (0.43857) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.30948 HOMO: -6.74026 LUMO: 2.14970 factor:1 | -1 (0.26452) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.59848 HOMO: -6.63686 LUMO: 2.17419 factor:1 | 1 (-1.02448) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76987 HOMO: -6.81917 LUMO: 2.10072 factor:1 | 1 (-0.19587) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53217 HOMO: -6.92802 LUMO: 2.04358 factor:1 | -1 (0.04182) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.49484 HOMO: -6.56067 LUMO: -0.47620 factor:1 | -1 (0.07916) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.14367 HOMO: -6.56611 LUMO: -0.77008 factor:1 | 1 (-0.56967) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93368 HOMO: -6.78380 LUMO: -0.64763 factor:1 | 1 (-0.35968) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78034 HOMO: -6.51985 LUMO: -0.24490 factor:1 | 1 (-0.20634) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85175 HOMO: -6.52529 LUMO: -0.27483 factor:1 | 1 (-0.27775) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.36298 HOMO: -7.10489 LUMO: -0.62586 factor:1 | -1 (1.21102) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.32320 HOMO: -7.18108 LUMO: 0.48980 factor:1 | -1 (1.25080) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61177 HOMO: -7.14299 LUMO: -0.63947 factor:1 | 1 (-0.03777) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84788 HOMO: -6.70761 LUMO: -0.54423 factor:1 | 1 (-0.27388) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.25870 HOMO: -7.32258 LUMO: -1.03675 factor:1 | -1 (0.31530) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.77046 HOMO: -6.65046 LUMO: -0.41361 factor:1 | 1 (-1.19646) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65255 HOMO: -6.76475 LUMO: -0.60137 factor:1 | 1 (-1.07855) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.86558 HOMO: -6.77836 LUMO: -0.54423 factor:1 | -1 (0.70842) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.03089 HOMO: -7.52395 LUMO: 0.26395 factor:1 | -1 (0.54311) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54950 HOMO: -6.93890 LUMO: -0.72382 factor:1 | 1 (-0.97550) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90382 HOMO: -6.72938 LUMO: -0.47348 factor:1 | 1 (-1.32982) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.47331 HOMO: -6.66951 LUMO: -0.40817 factor:1 | 1 (-0.89931) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.16608 HOMO: -6.60420 LUMO: -0.19320 factor:1 | 1 (-1.59208) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88949 HOMO: -6.67495 LUMO: -0.27211 factor:1 | 1 (-0.31549) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87575 HOMO: -7.23823 LUMO: -0.62858 factor:1 | 1 (-0.30175) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74297 HOMO: -7.27088 LUMO: 0.53334 factor:1 | 1 (-1.16897) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84276 HOMO: -7.20013 LUMO: 0.59049 factor:1 | 1 (-1.26876) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76551 HOMO: -6.60148 LUMO: -0.20953 factor:1 | 1 (-0.19151) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77659 HOMO: -6.69400 LUMO: -0.51974 factor:1 | 1 (-0.20259) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.42435 HOMO: -7.40422 LUMO: -0.98777 factor:1 | 1 (-1.85035) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90578 HOMO: -6.88176 LUMO: -0.71022 factor:1 | 1 (-1.33178) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97822 HOMO: -6.86271 LUMO: -0.59321 factor:1 | 1 (-1.40422) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.28938 HOMO: -6.73754 LUMO: -0.55239 factor:1 | 1 (-1.71538) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68665 HOMO: -6.71033 LUMO: 1.57010 factor:1 | 1 (-0.11266) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.79708 HOMO: -6.69672 LUMO: 1.68711 factor:1 | 1 (-0.22308) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.68057 HOMO: -6.67495 LUMO: 2.03813 factor:1 | 1 (-2.10657) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.97424 HOMO: -6.54434 LUMO: 1.83677 factor:1 | 1 (-1.40024) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66077 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-1.08677) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.74631 HOMO: -6.76747 LUMO: 1.87759 factor:1 | 1 (-2.17231) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.86708 HOMO: -6.58243 LUMO: 1.61364 factor:1 | 1 (-1.29309) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.15436 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-0.58036) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.07580 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-1.50180) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38596 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-0.81196) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41216 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-0.83817) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.40591 HOMO: -6.83278 LUMO: 1.91296 factor:1 | 1 (-0.83191) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52044 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-0.94644) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.54550 HOMO: -6.50080 LUMO: 1.73337 factor:1 | 1 (-0.97150) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50281 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-0.92881) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11834 HOMO: -6.63686 LUMO: 2.20140 factor:1 | 1 (-0.54434) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.48553 HOMO: -6.57427 LUMO: 1.87214 factor:1 | 1 (-0.91153) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44969 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-0.87569) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29627 HOMO: -6.63958 LUMO: 2.04902 factor:1 | 1 (-0.72227) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.70624 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-1.13224) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73493 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-0.16093) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67895 HOMO: -6.72938 LUMO: 2.28304 factor:1 | 1 (-0.10495) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80957 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-0.23557) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66173 HOMO: -6.95523 LUMO: 2.33474 factor:1 | 1 (-0.08773) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56641 HOMO: -6.59876 LUMO: 2.30480 factor:1 | -1 (0.00759) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.80105 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-0.22705) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.03054 HOMO: -7.06408 LUMO: 1.99187 factor:1 | -1 (1.54346) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54573 HOMO: -6.95795 LUMO: 1.88847 factor:1 | -1 (0.02827) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62714 HOMO: -6.85455 LUMO: 1.63813 factor:1 | 1 (-0.05314) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69329 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-0.11929) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39600 HOMO: -6.91441 LUMO: 1.68983 factor:1 | 1 (-0.82200) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.73631 HOMO: -6.89809 LUMO: 2.23678 factor:1 | 1 (-1.16231) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.58928 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-1.01528) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89310 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-1.31910) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.37233 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-0.79833) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39396 HOMO: -6.94979 LUMO: 2.28031 factor:1 | 1 (-0.81996) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06625 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-0.49225) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08919 HOMO: -6.87360 LUMO: 2.40277 factor:1 | 1 (-0.51519) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.50090 HOMO: -6.92802 LUMO: 1.89663 factor:1 | 1 (-0.92690) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.30846 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-0.73446) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28174 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-0.70774) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43967 HOMO: -6.54978 LUMO: 1.93201 factor:1 | 1 (-0.86568) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13134 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-0.55734) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.93333 HOMO: -6.55794 LUMO: 1.89663 factor:1 | -1 (0.64066) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.96163 HOMO: -6.07630 LUMO: 1.94289 factor:1 | -1 (0.61237) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.01260 HOMO: -7.46408 LUMO: 0.31565 factor:1 | -1 (0.56140) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.09430 HOMO: -6.63958 LUMO: -0.61770 factor:1 | 1 (-1.52030) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.82370 HOMO: -6.81101 LUMO: -0.57960 factor:1 | 1 (-2.24970) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.14278 HOMO: -6.74298 LUMO: -0.57960 factor:1 | -1 (0.43122) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.18359 HOMO: -6.63686 LUMO: -0.42994 factor:1 | 1 (-0.60959) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83381 HOMO: -6.60965 LUMO: -0.41089 factor:1 | 1 (-0.25981) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.93100 HOMO: -6.60692 LUMO: -0.80274 factor:1 | 1 (-1.35700) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.66144 HOMO: -6.58788 LUMO: -0.78097 factor:1 | -1 (0.91256) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.78097 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-0.20697) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.39662 HOMO: -6.63141 LUMO: -0.40545 factor:1 | -1 (1.17738) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.73244 HOMO: -6.62053 LUMO: -0.83811 factor:1 | -1 (1.84156) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.27060 HOMO: -6.59604 LUMO: -0.35375 factor:1 | -1 (1.30340) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05730 HOMO: -6.34297 LUMO: -0.39729 factor:1 | 1 (-0.48330) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75702 HOMO: -6.67223 LUMO: 1.97827 factor:1 | 1 (-0.18302) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.52350 HOMO: -6.40012 LUMO: 1.89935 factor:1 | -1 (1.05050) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01115 HOMO: -6.74842 LUMO: 1.97283 factor:1 | 1 (-0.43715) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.76933 HOMO: -6.76747 LUMO: 2.17147 factor:1 | -1 (0.80467) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.70220 HOMO: -6.72121 LUMO: 1.55649 factor:1 | -1 (0.87180) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.09129 HOMO: -6.97700 LUMO: 2.04085 factor:1 | 1 (-0.51729) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67525 HOMO: -7.06680 LUMO: 2.04085 factor:1 | 1 (-0.10125) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.31190 HOMO: -7.09673 LUMO: 2.35106 factor:1 | -1 (0.26210) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.75213 HOMO: -6.83006 LUMO: 2.14970 factor:1 | -1 (0.82187) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.32204 HOMO: -6.72665 LUMO: 2.20140 factor:1 | 1 (-0.74804) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83626 HOMO: -6.77291 LUMO: 2.34562 factor:1 | 1 (-0.26226) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22870 HOMO: -6.73754 LUMO: 2.00276 factor:1 | 1 (-0.65471) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.32468 HOMO: -7.04231 LUMO: 1.92112 factor:1 | 1 (-0.75068) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.51381 HOMO: -6.83822 LUMO: 1.72248 factor:1 | -1 (0.06019) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.57844 HOMO: -6.57971 LUMO: 2.16603 factor:1 | -1 (0.99556) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89068 HOMO: -6.80013 LUMO: 1.88575 factor:1 | 1 (-0.31669) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.96378 HOMO: -6.93618 LUMO: 2.18235 factor:1 | -1 (0.61022) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96927 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-0.39527) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.29021 HOMO: -7.06952 LUMO: 2.18507 factor:1 | -1 (0.28379) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.90110 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-1.32710) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.95536 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-1.38136) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01640 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-0.44240) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19124 HOMO: -7.17292 LUMO: 1.90752 factor:1 | -1 (0.38276) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.63921 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-2.06521) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91082 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-0.33682) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52017 HOMO: -6.85727 LUMO: 2.13609 factor:1 | 1 (-0.94617) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.51327 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-1.93927) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35687 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-0.78287) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.24523 HOMO: -6.67223 LUMO: 2.07351 factor:1 | -1 (0.32877) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.78373 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-2.20973) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39252 HOMO: -6.90897 LUMO: 2.28848 factor:1 | 1 (-0.81852) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55569 HOMO: -7.04231 LUMO: 1.70071 factor:1 | -1 (0.01831) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.51708 HOMO: -6.69944 LUMO: 1.94834 factor:1 | -1 (1.05692) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64830 HOMO: -6.56067 LUMO: 2.20956 factor:1 | 1 (-1.07431) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.40537 HOMO: -6.65046 LUMO: 2.06807 factor:1 | -1 (0.16863) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.92288 HOMO: -7.08584 LUMO: 1.98915 factor:1 | -1 (0.65111) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.00627 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-1.43227) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83330 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-0.25930) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89127 HOMO: -6.85183 LUMO: 2.16058 factor:1 | 1 (-1.31728) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86535 HOMO: -6.54706 LUMO: 1.92384 factor:1 | 1 (-0.29135) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83022 HOMO: -6.84366 LUMO: 2.48984 factor:1 | 1 (-0.25622) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.61655 HOMO: -6.77291 LUMO: 2.46263 factor:1 | 1 (-1.04255) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83025 HOMO: -7.01782 LUMO: 2.31025 factor:1 | 1 (-0.25625) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70655 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-0.13255) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66550 HOMO: -6.64230 LUMO: 1.97283 factor:1 | 1 (-1.09150) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94380 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-0.36980) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96013 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-0.38613) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38948 HOMO: -7.17020 LUMO: 2.06807 factor:1 | -1 (0.18452) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.31576 HOMO: -6.65046 LUMO: 2.20956 factor:1 | -1 (0.25824) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54186 HOMO: -7.07496 LUMO: 1.82861 factor:1 | -1 (0.03214) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.51598 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.94198) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.57377 HOMO: -6.92802 LUMO: 1.99187 factor:1 | 1 (-0.99977) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42800 HOMO: -6.69672 LUMO: 2.36739 factor:1 | 1 (-0.85400) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29148 HOMO: -7.13755 LUMO: 2.00276 factor:1 | 1 (-0.71748) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.55421 HOMO: -6.92530 LUMO: 2.25582 factor:1 | 1 (-0.98021) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.74929 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-1.17529) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.43671 HOMO: -6.87904 LUMO: 1.60003 factor:1 | 1 (-0.86271) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62429 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-0.05029) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.39774 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-0.82374) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.56308 HOMO: -6.74298 LUMO: 1.47486 factor:1 | 1 (-0.98908) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.36936 HOMO: -6.77019 LUMO: 1.90480 factor:1 | 1 (-0.79536) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53404 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-0.96004) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.46967 HOMO: -6.73482 LUMO: 2.08711 factor:1 | -1 (0.10433) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.09395 HOMO: -6.46543 LUMO: 1.73881 factor:1 | 1 (-1.51995) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44969 HOMO: -6.96067 LUMO: 2.26127 factor:1 | 1 (-0.87569) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.31409 HOMO: -6.67767 LUMO: 2.10616 factor:1 | 1 (-0.74010) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.40121 HOMO: -6.28855 LUMO: 2.35923 factor:1 | -1 (0.17279) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.42829 HOMO: -6.80285 LUMO: 1.62724 factor:1 | -1 (1.14571) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53625 HOMO: -6.85455 LUMO: 2.23133 factor:1 | 1 (-0.96225) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57269 HOMO: -6.51713 LUMO: 2.33474 factor:1 | -1 (0.00131) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.72449 HOMO: -6.88176 LUMO: 2.15242 factor:1 | -1 (0.84951) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76557 HOMO: -6.54434 LUMO: 2.32113 factor:1 | 1 (-0.19157) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54075 HOMO: -6.62597 LUMO: 2.24222 factor:1 | -1 (0.03325) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69713 HOMO: -6.74570 LUMO: 2.19868 factor:1 | 1 (-0.12313) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.82829 HOMO: -6.62869 LUMO: 1.98915 factor:1 | 1 (-0.25429) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50641 HOMO: -6.64502 LUMO: 2.13881 factor:1 | -1 (0.06759) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72870 HOMO: -6.95795 LUMO: 1.82316 factor:1 | 1 (-0.15470) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77621 HOMO: -6.77291 LUMO: 1.36329 factor:1 | 1 (-0.20221) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63721 HOMO: -6.45726 LUMO: 1.73064 factor:1 | 1 (-0.06321) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.58235 HOMO: -6.49264 LUMO: 1.77418 factor:1 | 1 (-0.00835) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.46621 HOMO: -6.60420 LUMO: 2.20956 factor:1 | -1 (0.10778) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74429 HOMO: -6.56067 LUMO: 2.05718 factor:1 | 1 (-0.17029) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.46806 HOMO: -6.62597 LUMO: 1.70343 factor:1 | -1 (0.10593) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.37590 HOMO: -6.69400 LUMO: 2.16875 factor:1 | -1 (0.19810) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.32861 HOMO: -6.63958 LUMO: 2.11977 factor:1 | -1 (0.24539) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66529 HOMO: -6.92802 LUMO: 1.82044 factor:1 | 1 (-0.09129) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.53079 HOMO: -6.56339 LUMO: 2.30480 factor:1 | -1 (0.04321) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.93527 HOMO: -6.63958 LUMO: 1.91024 factor:1 | -1 (1.63872) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.25841 HOMO: -6.93074 LUMO: 2.05446 factor:1 | -1 (1.31559) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.96509 HOMO: -6.61509 LUMO: 2.03813 factor:1 | -1 (0.60891) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.87072 HOMO: -6.61237 LUMO: 1.91296 factor:1 | -1 (0.70328) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47392 HOMO: -6.86815 LUMO: 1.95378 factor:1 | -1 (0.10008) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15021 HOMO: -6.63686 LUMO: 1.70888 factor:1 | -1 (0.42379) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.19772 HOMO: -6.57971 LUMO: 2.20140 factor:1 | -1 (0.37628) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.15149 HOMO: -6.41100 LUMO: 1.96738 factor:1 | -1 (0.42251) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70461 HOMO: -6.90081 LUMO: 1.65989 factor:1 | 1 (-0.13061) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38063 HOMO: -6.68312 LUMO: 1.97827 factor:1 | -1 (0.19336) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.63430 HOMO: -6.65318 LUMO: 2.10888 factor:1 | -1 (2.93970) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.65729 HOMO: -6.62053 LUMO: 2.28848 factor:1 | -1 (2.91671) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.84970 HOMO: -6.65863 LUMO: 2.29664 factor:1 | -1 (2.72430) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.88206 HOMO: -6.63958 LUMO: 2.07623 factor:1 | -1 (2.69194) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47661 HOMO: -6.58243 LUMO: 2.20684 factor:1 | -1 (0.09739) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73925 HOMO: -6.59332 LUMO: 2.05174 factor:1 | 1 (-0.16525) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.66429 HOMO: -6.95251 LUMO: 2.20140 factor:1 | 1 (-0.09029) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52175 HOMO: -6.84638 LUMO: 2.39732 factor:1 | -1 (0.05225) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.88373 HOMO: -6.86815 LUMO: 2.47896 factor:1 | -1 (0.69027) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45076 HOMO: -7.00693 LUMO: 2.43270 factor:1 | -1 (0.12324) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.78726 HOMO: -6.58788 LUMO: 2.30208 factor:1 | -1 (0.78674) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.85883 HOMO: -6.63958 LUMO: 2.28031 factor:1 | -1 (0.71517) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.80098 HOMO: -6.74570 LUMO: 2.28304 factor:1 | -1 (0.77302) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69324 HOMO: -6.78380 LUMO: 2.16331 factor:1 | 1 (-0.11924) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.06406 HOMO: -6.52529 LUMO: 2.05718 factor:1 | -1 (0.50994) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.12536 HOMO: -6.41644 LUMO: 1.65445 factor:1 | -1 (0.44863) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.07347 HOMO: -6.34570 LUMO: 1.22451 factor:1 | -1 (0.50053) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44534 HOMO: -6.14433 LUMO: 1.85582 factor:1 | -1 (0.12866) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71642 HOMO: -6.62053 LUMO: 1.92112 factor:1 | 1 (-0.14242) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.30692 HOMO: -6.63414 LUMO: 1.61908 factor:1 | -1 (3.26708) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.29622 HOMO: -6.75931 LUMO: 1.87214 factor:1 | -1 (3.27777) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.52594 HOMO: -6.55794 LUMO: 1.77418 factor:1 | -1 (3.04806) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.60254 HOMO: -6.52801 LUMO: 1.82044 factor:1 | -1 (2.97146) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.62168 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-2.04768) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.92347 HOMO: -6.93890 LUMO: 1.81228 factor:1 | 1 (-1.34947) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.34721 HOMO: -6.85455 LUMO: 1.75513 factor:1 | 1 (-0.77321) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.05977 HOMO: -6.86815 LUMO: 1.64629 factor:1 | 1 (-1.48577) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.10750 HOMO: -6.98516 LUMO: 1.84765 factor:1 | 1 (-1.53350) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60841 HOMO: -6.04637 LUMO: 1.94017 factor:1 | 1 (-1.03441) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.30372 HOMO: -6.86271 LUMO: 2.11977 factor:1 | 1 (-1.72972) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.49990 HOMO: -6.72938 LUMO: 2.11160 factor:1 | -1 (0.07410) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87501 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-0.30101) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.88618 HOMO: -6.18515 LUMO: 2.04630 factor:1 | 1 (-2.31218) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.22603 HOMO: -6.60965 LUMO: 2.17147 factor:1 | 1 (-1.65203) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.04826 HOMO: -6.87360 LUMO: 2.35378 factor:1 | 1 (-1.47426) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99767 HOMO: -6.72938 LUMO: 2.20140 factor:1 | 1 (-1.42367) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.29591 HOMO: -6.88448 LUMO: 2.54154 factor:1 | 1 (-1.72191) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.22448 HOMO: -6.87087 LUMO: 2.16058 factor:1 | 1 (-1.65048) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81972 HOMO: -7.11306 LUMO: 2.04085 factor:1 | 1 (-0.24572) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.13060 HOMO: -6.66951 LUMO: 1.68438 factor:1 | 1 (-1.55660) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.10712 HOMO: -7.08312 LUMO: 2.19324 factor:1 | 1 (-1.53312) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.41263 HOMO: -6.69128 LUMO: 2.13881 factor:1 | 1 (-0.83863) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.35920 HOMO: -6.80285 LUMO: 2.16603 factor:1 | 1 (-1.78520) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.66107 HOMO: -6.82189 LUMO: 2.46807 factor:1 | 1 (-1.08707) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.61201 HOMO: -6.78652 LUMO: 2.12521 factor:1 | 1 (-0.03801) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.54009 HOMO: -6.47903 LUMO: 1.70071 factor:1 | -1 (0.03391) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77550 HOMO: -6.37019 LUMO: 1.24356 factor:1 | 1 (-0.20150) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.21622 HOMO: -6.69400 LUMO: 1.67350 factor:1 | -1 (3.35778) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11945.73982 HOMO: -7.51851 LUMO: 0.27756 factor:1 | -1 (2.83417) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50594 HOMO: -6.95795 LUMO: -0.72110 factor:1 | -1 (0.06806) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.85042 HOMO: -6.88720 LUMO: -0.67484 factor:1 | -1 (0.72358) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.00378 HOMO: -6.83550 LUMO: -0.57144 factor:1 | -1 (0.57021) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.65991 HOMO: -6.80285 LUMO: -0.57144 factor:1 | -1 (0.91408) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.36197 HOMO: -6.76475 LUMO: -0.53062 factor:1 | -1 (0.21203) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.72125 HOMO: -6.66951 LUMO: 1.74969 factor:1 | -1 (0.85275) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.26950 HOMO: -6.53345 LUMO: 1.89935 factor:1 | -1 (0.30450) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.88969 HOMO: -6.65046 LUMO: 2.01364 factor:1 | -1 (0.68431) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.62888 HOMO: -6.64230 LUMO: 2.11977 factor:1 | 1 (-0.05489) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.95807 HOMO: -6.44910 LUMO: 2.13337 factor:1 | -1 (0.61593) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89137 HOMO: -7.05591 LUMO: 1.98915 factor:1 | -1 (0.68262) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.07095 HOMO: -7.02326 LUMO: 2.49256 factor:1 | -1 (1.50305) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11946.97353 HOMO: -6.32937 LUMO: 2.51161 factor:1 | -1 (1.60046) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.16880 HOMO: -6.96067 LUMO: 2.20140 factor:1 | -1 (1.40520) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.11609 HOMO: -6.97972 LUMO: 2.55243 factor:1 | -1 (1.45790) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.16482 HOMO: -6.72665 LUMO: 2.46535 factor:1 | -1 (0.40918) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.73738 HOMO: -6.41917 LUMO: 2.35106 factor:1 | -1 (0.83661) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.01769 HOMO: -6.75114 LUMO: 2.32929 factor:1 | -1 (0.55631) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.69412 HOMO: -6.91713 LUMO: 2.27215 factor:1 | -1 (0.87988) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.64968 HOMO: -6.54978 LUMO: 2.00276 factor:1 | -1 (0.92432) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.23750 HOMO: -6.62325 LUMO: 2.05990 factor:1 | -1 (0.33650) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89401 HOMO: -6.86271 LUMO: 2.14970 factor:1 | -1 (0.67999) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94944 HOMO: -6.77564 LUMO: 2.25855 factor:1 | -1 (0.62456) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68638 HOMO: -6.71305 LUMO: 1.94561 factor:1 | 1 (-0.11238) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47275 HOMO: -6.75659 LUMO: 1.94561 factor:1 | -1 (0.10125) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.32961 HOMO: -6.94979 LUMO: 2.33474 factor:1 | -1 (0.24439) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.55716 HOMO: -6.85727 LUMO: 2.50345 factor:1 | -1 (0.01684) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.59521 HOMO: -6.87360 LUMO: 2.43270 factor:1 | 1 (-2.02121) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.83560 HOMO: -6.57427 LUMO: 2.46807 factor:1 | 1 (-1.26160) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.89949 HOMO: -7.16204 LUMO: 2.15242 factor:1 | 1 (-1.32549) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.06894 HOMO: -6.62869 LUMO: 2.11432 factor:1 | 1 (-1.49494) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.13811 HOMO: -7.05591 LUMO: 2.26671 factor:1 | 1 (-1.56411) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.65519 HOMO: -7.13483 LUMO: 1.47758 factor:1 | 1 (-1.08119) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.98837 HOMO: -6.72938 LUMO: 1.57282 factor:1 | 1 (-1.41437) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.99773 HOMO: -6.17426 LUMO: 1.81228 factor:1 | 1 (-1.42373) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29502 HOMO: -6.65318 LUMO: 1.93473 factor:1 | 1 (-0.72102) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.42027 HOMO: -6.18515 LUMO: 2.01364 factor:1 | 1 (-0.84627) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.14491 HOMO: -7.05591 LUMO: 2.13337 factor:1 | 1 (-1.57091) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.46310 HOMO: -6.90897 LUMO: 2.29664 factor:1 | 1 (-0.88910) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44025 HOMO: -7.11034 LUMO: 2.17147 factor:1 | -1 (0.13374) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68951 HOMO: -6.82734 LUMO: 2.26671 factor:1 | 1 (-0.11551) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.77436 HOMO: -6.34842 LUMO: 2.34562 factor:1 | 1 (-0.20036) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60252 HOMO: -6.62053 LUMO: 2.22861 factor:1 | 1 (-0.02852) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.47906 HOMO: -6.80557 LUMO: 2.07079 factor:1 | -1 (0.09494) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.48815 HOMO: -6.60692 LUMO: 2.46263 factor:1 | -1 (0.08585) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70943 HOMO: -7.02054 LUMO: 2.08711 factor:1 | 1 (-0.13543) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.40991 HOMO: -6.78652 LUMO: 2.02453 factor:1 | -1 (0.16408) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68807 HOMO: -6.51168 LUMO: 2.06534 factor:1 | 1 (-0.11407) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.16197 HOMO: -6.50080 LUMO: 2.01636 factor:1 | 1 (-1.58797) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.52129 HOMO: -6.54434 LUMO: 1.84493 factor:1 | -1 (0.05271) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.33038 HOMO: -6.47087 LUMO: 1.76330 factor:1 | -1 (0.24362) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.45174 HOMO: -6.78924 LUMO: 2.39460 factor:1 | -1 (0.12226) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.50583 HOMO: -6.59876 LUMO: 1.84493 factor:1 | -1 (0.06816) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.68940 HOMO: -6.41644 LUMO: 2.05174 factor:1 | 1 (-0.11540) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.56195 HOMO: -6.52257 LUMO: 2.11160 factor:1 | -1 (1.01205) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.89320 HOMO: -6.90897 LUMO: 2.34018 factor:1 | -1 (0.68080) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.45244 HOMO: -6.97428 LUMO: 1.86126 factor:1 | 1 (-0.87844) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.65134 HOMO: -7.13483 LUMO: 2.14698 factor:1 | -1 (0.92266) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87357 HOMO: -7.16748 LUMO: 2.31841 factor:1 | 1 (-0.29957) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93790 HOMO: -6.87087 LUMO: 2.38916 factor:1 | 1 (-0.36390) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.83237 HOMO: -6.93074 LUMO: 2.42181 factor:1 | 1 (-0.25837) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01662 HOMO: -6.90081 LUMO: 2.00276 factor:1 | 1 (-0.44262) | 1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.19265 HOMO: -6.99333 LUMO: 2.03541 factor:1 | 1 (-0.61865) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.12125 HOMO: -6.89264 LUMO: 1.57554 factor:1 | 1 (-0.54725) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24405 HOMO: -6.48175 LUMO: 1.85854 factor:1 | 1 (-0.67005) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.59483 HOMO: -6.69400 LUMO: 1.62452 factor:1 | 1 (-2.02083) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.58248 HOMO: -6.50896 LUMO: 1.88303 factor:1 | 1 (-1.00848) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.64501 HOMO: -6.60420 LUMO: 2.05990 factor:1 | 1 (-1.07101) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.84616 HOMO: -7.14299 LUMO: 2.07351 factor:1 | 1 (-1.27216) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98016 HOMO: -7.06408 LUMO: 1.81228 factor:1 | 1 (-0.40616) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29877 HOMO: -6.67495 LUMO: 1.79595 factor:1 | 1 (-0.72478) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.44016 HOMO: -6.45182 LUMO: 2.15786 factor:1 | 1 (-0.86617) | -1 | -1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29208 HOMO: -6.93346 LUMO: 2.45719 factor:1 | 1 (-0.71808) | 1 | 1 |
| G: -5684.20830 HOMO: -6.56339 LUMO: 1.86126 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52735 HOMO: -6.50080 LUMO: 2.08167 factor:1 | 1 (-0.95335) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.62778 HOMO: -6.83550 LUMO: -0.67484 factor:1 | -1 (0.94622) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.44175 HOMO: -7.04231 LUMO: 0.54151 factor:1 | -1 (0.13225) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.37658 HOMO: -6.79740 LUMO: 1.91296 factor:1 | -1 (0.19742) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57732 HOMO: -7.35796 LUMO: -1.04220 factor:1 | 1 (-0.00332) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56472 HOMO: -6.62597 LUMO: -0.44082 factor:1 | -1 (0.00928) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.46175 HOMO: -6.45182 LUMO: -0.20409 factor:1 | -1 (0.11225) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.38099 HOMO: -6.51168 LUMO: -0.23130 factor:1 | -1 (0.19301) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59833 HOMO: -7.14027 LUMO: 0.49797 factor:1 | 1 (-0.02433) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.57101 HOMO: -7.55660 LUMO: 0.24762 factor:1 | -1 (0.00299) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.67942 HOMO: -6.88992 LUMO: -0.64763 factor:1 | -1 (0.89457) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11950.23457 HOMO: -6.72665 LUMO: -0.45987 factor:1 | 1 (-1.66057) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.35159 HOMO: -6.72121 LUMO: -0.58232 factor:1 | 1 (-0.77759) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52490 HOMO: -7.26816 LUMO: 0.32926 factor:1 | 1 (-0.95090) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.38952 HOMO: -6.57155 LUMO: -0.53606 factor:1 | 1 (-0.81553) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.59653 HOMO: -6.50896 LUMO: -0.43810 factor:1 | 1 (-0.02253) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.80764 HOMO: -6.73210 LUMO: -0.51430 factor:1 | -1 (0.76635) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.60169 HOMO: -6.77019 LUMO: -0.62858 factor:1 | 1 (-1.02769) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72938 HOMO: -6.82462 LUMO: -0.67484 factor:1 | 1 (-0.15538) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.02697 HOMO: -6.79740 LUMO: -0.55511 factor:1 | -1 (0.54703) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11947.94425 HOMO: -6.79740 LUMO: -0.67756 factor:1 | -1 (0.62975) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.08982 HOMO: -6.75114 LUMO: -0.55239 factor:1 | 1 (-0.51582) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97278 HOMO: -6.49536 LUMO: -0.25307 factor:1 | 1 (-0.39878) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07118 HOMO: -6.48992 LUMO: -0.25034 factor:1 | 1 (-0.49718) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.37586 HOMO: -6.52801 LUMO: -0.28028 factor:1 | 1 (-0.80187) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21782 HOMO: -7.22462 LUMO: 0.52518 factor:1 | 1 (-0.64382) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05727 HOMO: -6.59332 LUMO: -0.27211 factor:1 | 1 (-0.48327) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.69533 HOMO: -6.57427 LUMO: -0.16871 factor:1 | 1 (-0.12134) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.03161 HOMO: -6.71033 LUMO: 1.59187 factor:1 | 1 (-0.45761) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92181 HOMO: -6.72121 LUMO: 2.00004 factor:1 | 1 (-0.34782) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76940 HOMO: -6.61509 LUMO: 1.55921 factor:1 | 1 (-0.19540) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.88562 HOMO: -6.55250 LUMO: 1.73064 factor:1 | 1 (-0.31162) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13153 HOMO: -6.66135 LUMO: 2.02181 factor:1 | 1 (-0.55753) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.13964 HOMO: -6.84911 LUMO: 1.98099 factor:1 | 1 (-0.56564) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.24465 HOMO: -6.66679 LUMO: 1.98371 factor:1 | 1 (-0.67065) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06876 HOMO: -6.67495 LUMO: 2.04085 factor:1 | 1 (-0.49476) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.29284 HOMO: -6.89809 LUMO: 1.95106 factor:1 | 1 (-0.71884) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11741 HOMO: -6.50352 LUMO: 1.88847 factor:1 | 1 (-0.54341) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06960 HOMO: -6.93618 LUMO: 2.00004 factor:1 | 1 (-0.49560) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.94304 HOMO: -6.50896 LUMO: 1.73609 factor:1 | 1 (-0.36904) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02663 HOMO: -6.69672 LUMO: 2.37283 factor:1 | 1 (-0.45263) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28803 HOMO: -6.65591 LUMO: 2.20684 factor:1 | 1 (-0.71403) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06631 HOMO: -6.23957 LUMO: 1.78507 factor:1 | 1 (-0.49231) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.05899 HOMO: -6.35114 LUMO: 1.92112 factor:1 | 1 (-0.48499) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16849 HOMO: -6.53617 LUMO: 1.75241 factor:1 | 1 (-0.59449) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02489 HOMO: -6.60420 LUMO: 1.78779 factor:1 | 1 (-0.45089) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.28789 HOMO: -7.40422 LUMO: -0.97145 factor:1 | 1 (-0.71389) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.16824 HOMO: -6.80013 LUMO: -0.69117 factor:1 | 1 (-0.59424) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.23679 HOMO: -6.68040 LUMO: -0.47076 factor:1 | 1 (-0.66279) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.01618 HOMO: -7.20285 LUMO: -0.66124 factor:1 | 1 (-0.44219) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98818 HOMO: -6.82734 LUMO: -0.60137 factor:1 | 1 (-0.41418) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.86203 HOMO: -7.18653 LUMO: 0.59321 factor:1 | 1 (-0.28803) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.97901 HOMO: -7.29265 LUMO: 0.48164 factor:1 | 1 (-0.40501) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.53891 HOMO: -6.63414 LUMO: -0.25034 factor:1 | 1 (-0.96492) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.52702 HOMO: -7.20285 LUMO: 0.53879 factor:1 | 1 (-0.95302) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.98315 HOMO: -6.46815 LUMO: -0.21769 factor:1 | 1 (-0.40915) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.95967 HOMO: -6.57971 LUMO: -0.18776 factor:1 | 1 (-0.38567) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71604 HOMO: -6.90897 LUMO: 1.91296 factor:1 | 1 (-0.14204) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.91588 HOMO: -6.67495 LUMO: 2.04358 factor:1 | 1 (-0.34188) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.06457 HOMO: -6.94162 LUMO: 1.73881 factor:1 | 1 (-0.49057) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07999 HOMO: -6.73482 LUMO: 1.95922 factor:1 | 1 (-0.50600) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96582 HOMO: -6.70489 LUMO: 2.04358 factor:1 | 1 (-0.39182) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93237 HOMO: -7.04231 LUMO: 1.79323 factor:1 | 1 (-0.35837) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.07570 HOMO: -6.68584 LUMO: 1.60275 factor:1 | 1 (-0.50170) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.02995 HOMO: -6.40556 LUMO: 1.45581 factor:1 | 1 (-0.45595) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92247 HOMO: -6.94979 LUMO: 2.16603 factor:1 | 1 (-0.34847) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71199 HOMO: -6.84911 LUMO: 1.89935 factor:1 | 1 (-0.13799) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.37567 HOMO: -6.22052 LUMO: 1.57282 factor:1 | 1 (-0.80167) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.22985 HOMO: -6.51168 LUMO: 2.10072 factor:1 | 1 (-0.65585) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.93493 HOMO: -7.03686 LUMO: 2.12249 factor:1 | 1 (-0.36093) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.60663 HOMO: -6.84094 LUMO: 1.63268 factor:1 | 1 (-0.03263) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.92127 HOMO: -6.75387 LUMO: 1.72248 factor:1 | 1 (-0.34727) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.10114 HOMO: -6.86271 LUMO: 1.68711 factor:1 | 1 (-0.52714) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89792 HOMO: -6.84094 LUMO: 2.02997 factor:1 | 1 (-0.32392) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.21115 HOMO: -6.80557 LUMO: 2.02725 factor:1 | 1 (-0.63715) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89836 HOMO: -6.38651 LUMO: 1.53472 factor:1 | 1 (-0.32436) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.25096 HOMO: -7.51306 LUMO: 0.28572 factor:1 | 1 (-0.67696) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.11180 HOMO: -6.97972 LUMO: -0.74287 factor:1 | 1 (-0.53781) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.75757 HOMO: -6.83822 LUMO: -0.65852 factor:1 | 1 (-0.18357) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.65786 HOMO: -6.71305 LUMO: -0.49525 factor:1 | 1 (-0.08387) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.71838 HOMO: -6.60692 LUMO: -0.22313 factor:1 | 1 (-0.14438) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.63079 HOMO: -7.20013 LUMO: 0.55239 factor:1 | 1 (-0.05679) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.58369 HOMO: -6.60420 LUMO: -0.28028 factor:1 | 1 (-0.00969) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.67395 HOMO: -6.69128 LUMO: -0.30477 factor:1 | 1 (-0.09995) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.20397 HOMO: -6.65591 LUMO: -0.25579 factor:1 | 1 (-0.62997) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.96911 HOMO: -6.69128 LUMO: 1.70888 factor:1 | 1 (-0.39511) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11949.27505 HOMO: -6.50080 LUMO: 1.87759 factor:1 | 1 (-0.70105) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.72565 HOMO: -6.85727 LUMO: 1.99187 factor:1 | 1 (-0.15165) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.81057 HOMO: -6.58788 LUMO: 1.79051 factor:1 | 1 (-0.23658) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.85398 HOMO: -6.64230 LUMO: 2.16058 factor:1 | 1 (-0.27998) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.76200 HOMO: -6.58788 LUMO: 2.10616 factor:1 | 1 (-0.18800) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.87942 HOMO: -7.01782 LUMO: 2.13609 factor:1 | 1 (-0.30542) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.73114 HOMO: -6.31304 LUMO: 2.31841 factor:1 | 1 (-0.15715) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.70750 HOMO: -6.94979 LUMO: 2.07895 factor:1 | 1 (-0.13350) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.56423 HOMO: -6.88992 LUMO: 2.28031 factor:1 | -1 (0.00977) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.64812 HOMO: -6.66407 LUMO: 2.07623 factor:1 | 1 (-0.07412) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.89648 HOMO: -6.52529 LUMO: 1.70071 factor:1 | 1 (-0.32248) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.74589 HOMO: -6.58788 LUMO: 1.57282 factor:1 | 1 (-0.17189) | -1 | -1 |
| G: -5684.20830 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -11948.84851 HOMO: -6.55250 LUMO: 1.95378 factor:1 | 1 (-0.27451) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.28943 HOMO: -6.24773 LUMO: 1.77962 factor:1 | -1 (1.88529) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.16649 HOMO: -6.31304 LUMO: 2.18507 factor:1 | -1 (2.00823) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.23329 HOMO: -6.18243 LUMO: 2.01636 factor:1 | -1 (0.94143) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.91486 HOMO: -6.99877 LUMO: 2.14970 factor:1 | -1 (1.25986) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.17222 HOMO: -6.72665 LUMO: 2.07079 factor:1 | -1 (1.00249) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.36007 HOMO: -6.36202 LUMO: 2.17419 factor:1 | -1 (0.81465) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.01326 HOMO: -6.78652 LUMO: 2.05718 factor:1 | -1 (1.16146) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.58891 HOMO: -6.87360 LUMO: 2.34290 factor:1 | -1 (0.58581) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.23116 HOMO: -6.62053 LUMO: 1.89391 factor:1 | -1 (0.94355) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.57895 HOMO: -6.58788 LUMO: 1.83133 factor:1 | -1 (0.59577) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.44815 HOMO: -7.08584 LUMO: 1.91568 factor:1 | -1 (0.72657) | 1 | 1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.26737 HOMO: -6.56883 LUMO: 1.81228 factor:1 | 1 (-0.09265) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.31484 HOMO: -6.66135 LUMO: 1.92384 factor:1 | -1 (0.85988) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.11682 HOMO: -6.64502 LUMO: 2.15786 factor:1 | -1 (1.05790) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.42796 HOMO: -6.71305 LUMO: 1.91840 factor:1 | -1 (0.74676) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.09085 HOMO: -6.44094 LUMO: 1.74425 factor:1 | -1 (0.08387) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.83924 HOMO: -6.51985 LUMO: 1.84221 factor:1 | -1 (1.33548) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.46467 HOMO: -6.63414 LUMO: -0.24762 factor:1 | -1 (0.71005) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.37246 HOMO: -6.60420 LUMO: -0.22585 factor:1 | 1 (-0.19775) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.67588 HOMO: -7.19741 LUMO: 0.58232 factor:1 | -1 (0.49884) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.23516 HOMO: -6.77019 LUMO: -0.56872 factor:1 | 1 (-0.06044) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.48254 HOMO: -7.46136 LUMO: 0.28844 factor:1 | -1 (0.69218) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12383.43497 HOMO: -6.60420 LUMO: -0.54151 factor:1 | -1 (2.73975) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12383.73723 HOMO: -6.53890 LUMO: -0.46531 factor:1 | -1 (2.43749) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.40704 HOMO: -6.81645 LUMO: -0.57144 factor:1 | -1 (1.76768) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.06614 HOMO: -7.48041 LUMO: 0.28572 factor:1 | -1 (2.10858) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.24442 HOMO: -6.75659 LUMO: -0.45715 factor:1 | -1 (0.93030) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.18716 HOMO: -6.66135 LUMO: -0.41906 factor:1 | -1 (0.98756) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.35705 HOMO: -6.55794 LUMO: -0.27483 factor:1 | -1 (1.81767) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.23925 HOMO: -7.07496 LUMO: -0.63403 factor:1 | -1 (0.93547) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.44380 HOMO: -7.12394 LUMO: 0.53334 factor:1 | -1 (1.73092) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.39933 HOMO: -6.53617 LUMO: -0.25579 factor:1 | -1 (0.77539) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.22261 HOMO: -6.50896 LUMO: -0.25034 factor:1 | 1 (-0.04789) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.39324 HOMO: -7.17564 LUMO: -0.68573 factor:1 | -1 (0.78148) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12382.74301 HOMO: -6.53617 LUMO: -0.30749 factor:1 | -1 (3.43171) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12383.44781 HOMO: -6.55522 LUMO: -0.30749 factor:1 | -1 (2.72691) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12383.44830 HOMO: -7.05591 LUMO: -0.71022 factor:1 | -1 (2.72642) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.08635 HOMO: -7.17564 LUMO: -0.69933 factor:1 | -1 (1.08837) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.87295 HOMO: -6.78380 LUMO: -0.67756 factor:1 | -1 (0.30177) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.35947 HOMO: -6.62325 LUMO: 2.02725 factor:1 | -1 (0.81525) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.06436 HOMO: -6.63414 LUMO: 1.91296 factor:1 | -1 (1.11036) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12383.82308 HOMO: -6.83278 LUMO: 1.65717 factor:1 | -1 (2.35164) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12382.24978 HOMO: -6.66407 LUMO: 1.95650 factor:1 | -1 (3.92494) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12383.43067 HOMO: -6.61237 LUMO: 2.11432 factor:1 | -1 (2.74405) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12383.34433 HOMO: -6.62053 LUMO: 2.09256 factor:1 | -1 (2.83039) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12383.52692 HOMO: -6.78652 LUMO: 2.13609 factor:1 | -1 (2.64780) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12383.33614 HOMO: -6.94707 LUMO: 1.81772 factor:1 | -1 (2.83858) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.10333 HOMO: -6.85183 LUMO: 2.12793 factor:1 | -1 (1.07139) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.34971 HOMO: -6.81101 LUMO: 1.83949 factor:1 | -1 (1.82501) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.13644 HOMO: -6.98788 LUMO: 2.16058 factor:1 | -1 (1.03828) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.95580 HOMO: -6.62869 LUMO: 2.00820 factor:1 | -1 (0.21892) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.12316 HOMO: -6.34025 LUMO: 2.25855 factor:1 | -1 (1.05156) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.06882 HOMO: -6.01372 LUMO: 2.01636 factor:1 | -1 (1.10590) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.16975 HOMO: -6.89264 LUMO: 2.27487 factor:1 | -1 (1.00497) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.24956 HOMO: -6.53073 LUMO: 2.20684 factor:1 | -1 (0.92516) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.26327 HOMO: -6.83278 LUMO: 1.53744 factor:1 | -1 (0.91145) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.82087 HOMO: -6.41917 LUMO: 1.82316 factor:1 | -1 (1.35385) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.93519 HOMO: -6.56339 LUMO: 1.63813 factor:1 | -1 (1.23953) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.54148 HOMO: -6.88992 LUMO: 1.65173 factor:1 | -1 (0.63324) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.30969 HOMO: -6.63141 LUMO: 1.92112 factor:1 | 1 (-0.13497) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.03376 HOMO: -6.83822 LUMO: 1.88847 factor:1 | -1 (0.14095) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.30202 HOMO: -6.84638 LUMO: 1.90480 factor:1 | -1 (0.87270) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.12251 HOMO: -6.82462 LUMO: 1.70888 factor:1 | -1 (1.05221) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.11908 HOMO: -6.82734 LUMO: 2.12521 factor:1 | -1 (1.05564) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.98296 HOMO: -6.94435 LUMO: 1.87214 factor:1 | -1 (0.19176) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.34255 HOMO: -6.98516 LUMO: 2.51433 factor:1 | -1 (1.83217) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.25409 HOMO: -6.74026 LUMO: 2.15514 factor:1 | -1 (1.92063) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.24757 HOMO: -6.93618 LUMO: 2.54426 factor:1 | -1 (0.92715) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.11901 HOMO: -6.28583 LUMO: 2.53610 factor:1 | -1 (2.05571) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12382.37163 HOMO: -6.56883 LUMO: 1.94834 factor:1 | -1 (3.80309) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.61566 HOMO: -7.08584 LUMO: 1.99187 factor:1 | -1 (0.55906) | 1 | 1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.93306 HOMO: -6.19059 LUMO: 1.99732 factor:1 | -1 (1.24166) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.53371 HOMO: -6.78108 LUMO: 2.03813 factor:1 | -1 (1.64101) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.59953 HOMO: -6.82189 LUMO: 1.77418 factor:1 | -1 (1.57519) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.61841 HOMO: -6.45454 LUMO: 1.78779 factor:1 | -1 (0.55631) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.69962 HOMO: -6.84366 LUMO: 1.77690 factor:1 | -1 (1.47510) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.39431 HOMO: -6.74026 LUMO: 1.67622 factor:1 | -1 (1.78041) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.51582 HOMO: -6.76475 LUMO: 2.40277 factor:1 | -1 (0.65890) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.35503 HOMO: -6.65863 LUMO: 1.86670 factor:1 | -1 (0.81969) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.34134 HOMO: -6.50080 LUMO: 1.93201 factor:1 | -1 (0.83338) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12383.30430 HOMO: -6.34842 LUMO: 1.70888 factor:1 | -1 (2.87042) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12383.37668 HOMO: -6.60692 LUMO: 2.20140 factor:1 | -1 (2.79804) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.00243 HOMO: -6.74026 LUMO: 2.14970 factor:1 | -1 (1.17229) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.15007 HOMO: -6.63686 LUMO: 2.17419 factor:1 | -1 (1.02464) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.02022 HOMO: -6.81917 LUMO: 2.10072 factor:1 | -1 (1.15450) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.01214 HOMO: -6.92802 LUMO: 2.04358 factor:1 | -1 (1.16258) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.21153 HOMO: -6.56067 LUMO: -0.47620 factor:1 | -1 (1.96319) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.12633 HOMO: -6.56611 LUMO: -0.77008 factor:1 | -1 (2.04839) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.07041 HOMO: -6.78380 LUMO: -0.64763 factor:1 | -1 (2.10431) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12383.29382 HOMO: -6.51985 LUMO: -0.24490 factor:1 | -1 (2.88090) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12383.26890 HOMO: -6.52529 LUMO: -0.27483 factor:1 | -1 (2.90582) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12383.58324 HOMO: -7.10489 LUMO: -0.62586 factor:1 | -1 (2.59148) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12383.06854 HOMO: -7.18108 LUMO: 0.48980 factor:1 | -1 (3.10618) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.08543 HOMO: -7.14299 LUMO: -0.63947 factor:1 | -1 (2.08929) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.30609 HOMO: -6.70761 LUMO: -0.54423 factor:1 | -1 (1.86863) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.20559 HOMO: -7.32258 LUMO: -1.03675 factor:1 | -1 (1.96912) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.12369 HOMO: -6.65046 LUMO: -0.41361 factor:1 | -1 (2.05103) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12383.93754 HOMO: -6.76475 LUMO: -0.60137 factor:1 | -1 (2.23718) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12383.63737 HOMO: -6.77836 LUMO: -0.54423 factor:1 | -1 (2.53735) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.35656 HOMO: -7.52395 LUMO: 0.26395 factor:1 | -1 (1.81816) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12381.96561 HOMO: -6.93890 LUMO: -0.72382 factor:1 | -1 (4.20911) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12382.18643 HOMO: -6.72938 LUMO: -0.47348 factor:1 | -1 (3.98829) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.90656 HOMO: -6.66951 LUMO: -0.40817 factor:1 | -1 (1.26816) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12385.50804 HOMO: -6.60420 LUMO: -0.19320 factor:1 | -1 (0.66668) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12383.67427 HOMO: -6.67495 LUMO: -0.27211 factor:1 | -1 (2.50045) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.21868 HOMO: -7.23823 LUMO: -0.62858 factor:1 | -1 (1.95604) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.09112 HOMO: -7.27088 LUMO: 0.53334 factor:1 | -1 (2.08360) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.03574 HOMO: -7.20013 LUMO: 0.59049 factor:1 | -1 (2.13898) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12383.07578 HOMO: -6.60148 LUMO: -0.20953 factor:1 | -1 (3.09894) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.01101 HOMO: -6.69400 LUMO: -0.51974 factor:1 | -1 (2.16371) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12383.24114 HOMO: -7.40422 LUMO: -0.98777 factor:1 | -1 (2.93358) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12382.31234 HOMO: -6.88176 LUMO: -0.71022 factor:1 | -1 (3.86238) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12382.82111 HOMO: -6.86271 LUMO: -0.59321 factor:1 | -1 (3.35361) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12383.19290 HOMO: -6.73754 LUMO: -0.55239 factor:1 | -1 (2.98182) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12383.14873 HOMO: -6.71033 LUMO: 1.57010 factor:1 | -1 (3.02599) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12383.21763 HOMO: -6.69672 LUMO: 1.68711 factor:1 | -1 (2.95709) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12383.23026 HOMO: -6.67495 LUMO: 2.03813 factor:1 | -1 (2.94446) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12383.23339 HOMO: -6.54434 LUMO: 1.83677 factor:1 | -1 (2.94133) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.84173 HOMO: -6.57155 LUMO: 1.77146 factor:1 | 1 (-0.66701) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.13925 HOMO: -6.76747 LUMO: 1.87759 factor:1 | 1 (-0.96453) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.42515 HOMO: -6.58243 LUMO: 1.61364 factor:1 | 1 (-0.25043) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.40285 HOMO: -6.61781 LUMO: 2.13881 factor:1 | 1 (-1.22813) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.86594 HOMO: -6.62597 LUMO: 2.00276 factor:1 | 1 (-0.69122) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.09993 HOMO: -7.01237 LUMO: 1.95922 factor:1 | 1 (-0.92521) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.86026 HOMO: -7.03959 LUMO: 2.16875 factor:1 | 1 (-0.68554) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.85930 HOMO: -6.83278 LUMO: 1.91296 factor:1 | 1 (-0.68458) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.20483 HOMO: -6.40012 LUMO: 1.95650 factor:1 | 1 (-1.03011) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.78728 HOMO: -6.50080 LUMO: 1.73337 factor:1 | 1 (-0.61256) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.34840 HOMO: -6.95795 LUMO: 2.28848 factor:1 | 1 (-1.17368) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.01487 HOMO: -6.63686 LUMO: 2.20140 factor:1 | 1 (-0.84015) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.24225 HOMO: -6.57427 LUMO: 1.87214 factor:1 | 1 (-1.06753) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.87490 HOMO: -6.38379 LUMO: 2.32113 factor:1 | 1 (-0.70018) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.01427 HOMO: -6.63958 LUMO: 2.04902 factor:1 | 1 (-0.83955) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.63214 HOMO: -6.70216 LUMO: 1.93201 factor:1 | 1 (-0.45742) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.69258 HOMO: -6.80557 LUMO: 2.23678 factor:1 | 1 (-0.51786) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.69279 HOMO: -6.72938 LUMO: 2.28304 factor:1 | 1 (-1.51807) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.65682 HOMO: -6.56067 LUMO: 1.66806 factor:1 | 1 (-0.48210) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.19496 HOMO: -6.95523 LUMO: 2.33474 factor:1 | 1 (-1.02024) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.09251 HOMO: -6.59876 LUMO: 2.30480 factor:1 | -1 (0.08221) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.06072 HOMO: -6.87360 LUMO: 1.75786 factor:1 | 1 (-0.88600) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.44350 HOMO: -7.06408 LUMO: 1.99187 factor:1 | 1 (-1.26879) | 1 | 1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.26266 HOMO: -6.95795 LUMO: 1.88847 factor:1 | 1 (-1.08794) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.04880 HOMO: -6.85455 LUMO: 1.63813 factor:1 | 1 (-0.87408) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.62874 HOMO: -7.09129 LUMO: 2.31569 factor:1 | 1 (-0.45402) | 1 | 1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.59579 HOMO: -6.91441 LUMO: 1.68983 factor:1 | 1 (-0.42107) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.54586 HOMO: -6.89809 LUMO: 2.23678 factor:1 | 1 (-0.37114) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.66360 HOMO: -6.78652 LUMO: 1.98371 factor:1 | 1 (-0.48888) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.65696 HOMO: -6.94707 LUMO: 2.23678 factor:1 | 1 (-0.48224) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.59195 HOMO: -7.07224 LUMO: 2.13337 factor:1 | 1 (-0.41723) | 1 | 1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.60833 HOMO: -6.94979 LUMO: 2.28031 factor:1 | 1 (-0.43361) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.69525 HOMO: -6.60965 LUMO: 2.20412 factor:1 | 1 (-0.52053) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.63421 HOMO: -6.87360 LUMO: 2.40277 factor:1 | 1 (-0.45949) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.70042 HOMO: -6.92802 LUMO: 1.89663 factor:1 | 1 (-0.52570) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.61459 HOMO: -6.88448 LUMO: 2.02725 factor:1 | 1 (-0.43987) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.71704 HOMO: -6.69128 LUMO: 1.55105 factor:1 | 1 (-0.54232) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.76034 HOMO: -6.54978 LUMO: 1.93201 factor:1 | 1 (-0.58562) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.79587 HOMO: -6.19331 LUMO: 1.46941 factor:1 | 1 (-0.62115) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.72449 HOMO: -6.55794 LUMO: 1.89663 factor:1 | 1 (-1.54977) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.68354 HOMO: -6.07630 LUMO: 1.94289 factor:1 | 1 (-1.50882) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.66443 HOMO: -7.46408 LUMO: 0.31565 factor:1 | 1 (-1.48971) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.73603 HOMO: -6.63958 LUMO: -0.61770 factor:1 | 1 (-1.56131) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.14793 HOMO: -6.81101 LUMO: -0.57960 factor:1 | 1 (-0.97322) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.43796 HOMO: -6.74298 LUMO: -0.57960 factor:1 | 1 (-0.26324) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.44237 HOMO: -6.63686 LUMO: -0.42994 factor:1 | 1 (-0.26765) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.50686 HOMO: -6.60965 LUMO: -0.41089 factor:1 | 1 (-0.33214) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.24957 HOMO: -6.60692 LUMO: -0.80274 factor:1 | 1 (-1.07485) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.42522 HOMO: -6.58788 LUMO: -0.78097 factor:1 | 1 (-1.25050) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.39587 HOMO: -6.67767 LUMO: -0.48436 factor:1 | 1 (-0.22115) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.43287 HOMO: -6.63141 LUMO: -0.40545 factor:1 | 1 (-0.25815) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.34759 HOMO: -6.62053 LUMO: -0.83811 factor:1 | 1 (-0.17287) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.50310 HOMO: -6.59604 LUMO: -0.35375 factor:1 | 1 (-1.32838) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.57350 HOMO: -6.34297 LUMO: -0.39729 factor:1 | 1 (-0.39878) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.63633 HOMO: -6.67223 LUMO: 1.97827 factor:1 | 1 (-0.46161) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.42313 HOMO: -6.40012 LUMO: 1.89935 factor:1 | 1 (-0.24841) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.36153 HOMO: -6.74842 LUMO: 1.97283 factor:1 | 1 (-0.18681) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.47440 HOMO: -6.76747 LUMO: 2.17147 factor:1 | 1 (-0.29968) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.76616 HOMO: -6.72121 LUMO: 1.55649 factor:1 | 1 (-0.59144) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.89013 HOMO: -6.97700 LUMO: 2.04085 factor:1 | 1 (-0.71541) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.87495 HOMO: -7.06680 LUMO: 2.04085 factor:1 | 1 (-0.70023) | 1 | 1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.21554 HOMO: -7.09673 LUMO: 2.35106 factor:1 | 1 (-0.04082) | 1 | 1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.06065 HOMO: -6.83006 LUMO: 2.14970 factor:1 | -1 (0.11407) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.18789 HOMO: -6.72665 LUMO: 2.20140 factor:1 | 1 (-0.01317) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.11066 HOMO: -6.77291 LUMO: 2.34562 factor:1 | -1 (0.06406) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.44841 HOMO: -6.73754 LUMO: 2.00276 factor:1 | 1 (-0.27369) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.51418 HOMO: -7.04231 LUMO: 1.92112 factor:1 | 1 (-0.33946) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.27731 HOMO: -6.83822 LUMO: 1.72248 factor:1 | 1 (-0.10259) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12384.28070 HOMO: -6.57971 LUMO: 2.16603 factor:1 | -1 (1.89402) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.41217 HOMO: -6.80013 LUMO: 1.88575 factor:1 | 1 (-0.23745) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.89846 HOMO: -6.93618 LUMO: 2.18235 factor:1 | 1 (-0.72374) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.61035 HOMO: -6.54706 LUMO: 1.91024 factor:1 | 1 (-0.43563) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.50462 HOMO: -7.06952 LUMO: 2.18507 factor:1 | 1 (-1.32990) | 1 | 1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.26086 HOMO: -7.05047 LUMO: 1.82044 factor:1 | 1 (-1.08614) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.12233 HOMO: -6.87632 LUMO: 1.92657 factor:1 | 1 (-0.94761) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.04747 HOMO: -6.58788 LUMO: 1.91568 factor:1 | 1 (-0.87275) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.33488 HOMO: -7.17292 LUMO: 1.90752 factor:1 | 1 (-1.16016) | 1 | 1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.25477 HOMO: -6.93890 LUMO: 1.80684 factor:1 | 1 (-1.08005) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.32587 HOMO: -7.10761 LUMO: 2.20956 factor:1 | 1 (-1.15115) | 1 | 1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.46897 HOMO: -6.85727 LUMO: 2.13609 factor:1 | 1 (-1.29426) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.04627 HOMO: -6.64502 LUMO: 1.38506 factor:1 | 1 (-0.87155) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.24046 HOMO: -6.87360 LUMO: 1.15648 factor:1 | 1 (-0.06574) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.34416 HOMO: -6.67223 LUMO: 2.07351 factor:1 | 1 (-0.16945) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.91710 HOMO: -6.29671 LUMO: 2.43270 factor:1 | 1 (-0.74238) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.88896 HOMO: -6.90897 LUMO: 2.28848 factor:1 | 1 (-0.71424) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.98458 HOMO: -7.04231 LUMO: 1.70071 factor:1 | 1 (-0.80987) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.16158 HOMO: -6.69944 LUMO: 1.94834 factor:1 | -1 (0.01314) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.21216 HOMO: -6.56067 LUMO: 2.20956 factor:1 | 1 (-0.03744) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.74148 HOMO: -6.65046 LUMO: 2.06807 factor:1 | 1 (-0.56676) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.21445 HOMO: -7.08584 LUMO: 1.98915 factor:1 | 1 (-0.03973) | 1 | 1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.89511 HOMO: -6.69400 LUMO: 2.09256 factor:1 | 1 (-0.72039) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.57497 HOMO: -6.62869 LUMO: 2.16331 factor:1 | 1 (-0.40025) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.45045 HOMO: -6.85183 LUMO: 2.16058 factor:1 | 1 (-0.27573) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.57244 HOMO: -6.54706 LUMO: 1.92384 factor:1 | 1 (-0.39772) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.54179 HOMO: -6.84366 LUMO: 2.48984 factor:1 | 1 (-1.36707) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.01019 HOMO: -6.77291 LUMO: 2.46263 factor:1 | 1 (-0.83547) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.96589 HOMO: -7.01782 LUMO: 2.31025 factor:1 | 1 (-0.79117) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.59655 HOMO: -6.94707 LUMO: 2.29664 factor:1 | 1 (-0.42183) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.75040 HOMO: -6.64230 LUMO: 1.97283 factor:1 | 1 (-0.57568) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.76629 HOMO: -6.47359 LUMO: 2.20412 factor:1 | 1 (-1.59157) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.75111 HOMO: -6.90625 LUMO: 1.92384 factor:1 | 1 (-0.57639) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.67573 HOMO: -7.17020 LUMO: 2.06807 factor:1 | 1 (-1.50101) | 1 | 1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.77062 HOMO: -6.65046 LUMO: 2.20956 factor:1 | 1 (-0.59590) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.75646 HOMO: -7.07496 LUMO: 1.82861 factor:1 | 1 (-1.58174) | 1 | 1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.75163 HOMO: -6.83006 LUMO: 2.14970 factor:1 | 1 (-0.57691) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.71894 HOMO: -6.92802 LUMO: 1.99187 factor:1 | 1 (-1.54422) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.56821 HOMO: -6.69672 LUMO: 2.36739 factor:1 | 1 (-1.39350) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.57886 HOMO: -7.13755 LUMO: 2.00276 factor:1 | 1 (-0.40414) | 1 | 1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.46897 HOMO: -6.92530 LUMO: 2.25582 factor:1 | 1 (-1.29426) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.45997 HOMO: -6.77564 LUMO: 1.97827 factor:1 | 1 (-1.28525) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12386.48387 HOMO: -6.87904 LUMO: 1.60003 factor:1 | 1 (-0.30915) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.12146 HOMO: -6.62869 LUMO: 1.90480 factor:1 | 1 (-0.94674) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.27496 HOMO: -6.71033 LUMO: 1.54833 factor:1 | 1 (-1.10024) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.55921 HOMO: -6.74298 LUMO: 1.47486 factor:1 | 1 (-1.38449) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.03865 HOMO: -6.77019 LUMO: 1.90480 factor:1 | 1 (-0.86393) | -1 | -1 |
| G: -6121.80903 HOMO: -7.05319 LUMO: 1.54016 factor:1 | G: -6264.36569 HOMO: -7.05863 LUMO: 1.58914 factor:1 | G: -12387.19392 HOMO: -6.70489 LUMO: 1.99459 factor:1 | 1 (-1.01920) | -1 | -1 |