

Supplementary Material

B3LYP/6-31++G TBP constrained geometry**

6	1.57204	-0.61655	1.26053
6	0.43697	-1.48757	1.24412
6	0.31358	-2.02978	-0.06268
6	1.38164	-1.50964	-0.86054
6	2.15793	-0.65266	-0.04004
1	1.9334	-0.05299	2.10927
1	-0.23249	-1.67331	2.07296
1	-0.44024	-2.73203	-0.39036
1	1.55958	-1.72305	-1.90616
1	3.02848	-0.093	-0.35625
25	0.13144	0.13105	-0.13964
6	0.82464	1.71355	-0.73569
6	-0.90052	1.00796	1.04318
8	-1.47557	1.5511	1.89101
8	1.32935	2.69683	-1.07396
14	-2.29326	-0.50929	-0.84681
1	-2.06857	0.15143	-2.21539
1	-2.51582	-1.16377	0.50885
1	-2.5579	-1.83585	-1.53072
1	-3.43472	0.44114	-0.57539

B3LYP/6-31++G** fully optimised geometry

1	-2.014803	-2.272621	.207775
14	-1.744818	-1.328543	-.915901
25	.033416	.126973	-.087601
1	-1.405677	-2.196578	-2.081025
1	-.651632	-.124147	-1.472191
1	-3.021414	-.635673	-1.226525
8	-1.985258	.525381	2.029709
6	-.213397	1.820759	-.658251
6	-1.224343	.366345	1.166997
8	-.344322	2.915686	-1.011059
1	1.995253	1.027125	1.854124
6	1.832899	.275690	1.094150
6	2.183861	.380964	-.285454
1	.868400	-1.400250	2.226738
1	2.644038	1.238492	-.757962
6	1.803230	-.819409	-.938168
1	1.921379	-1.036218	-1.990851
6	1.216356	-1.684593	.037590
1	.854062	-2.688603	-.136287
6	1.241242	-1.008886	1.289746