Supplementary information (ESI) for Phys. Chem. Chem. Phys.

This file contains Cartesian coordinates for Di, Cy, Di/Di, Cy/Cy, Di/Cy, Tz/Tz and Tz/Bz optimized at the MP2/DZP++ level of theory.

Di

C	0.00000000	0.00000000	0.69232000
C	0.00000000	0.00000000	-0.69232000
C	0.00000000	0.00000000	1.92741600
C	0.00000000	0.00000000	-1.92741600
H	0.00000000	0.00000000	2.99804000
H	0.00000000	0.00000000	-2.99804000

Cy

C	0.6956842407	0.0000000000	0.0000000000
C	-0.6956842407	0.0000000000	0.0000000000
N	1.8886357750	0.0000000000	0.0000000000
N	-1.8886357750	0.0000000000	0.0000000000

Di/Di

C	-0.07341700	1.71353300	0.00000000
C	1.28546800	1.97312200	0.00000000
C	-1.28546800	1.47389300	0.00000000
C	2.49902300	2.20666500	0.00000000
C	-1.28546800	-1.97312200	0.00000000
C	0.07341700	-1.71353300	0.00000000
C	-2.49902300	-2.20666500	0.00000000
C	1.28546800	-1.47389300	0.00000000
H	-3.54650500	-2.42846400	0.00000000
H	2.33475100	-1.26177000	0.00000000
H	-2.33475100	1.26177000	0.00000000
H	3.54650500	2.42846400	0.00000000

Cy/Cy

C	0.5483608130	1.6645431609	0.0000000000
C	1.9350277751	1.7733567164	0.0000000000
C	-1.9350277751	-1.7733567164	0.0000000000
C	-0.5483608130	-1.6645431609	0.0000000000
N	-3.1235996933	-1.8777924126	0.0000000000
N	0.6407287091	-1.5665637536	0.0000000000
N	3.1235996933	1.8777924126	0.0000000000
N	-0.6407287091	1.5665637536	0.0000000000

Di/Cy

C	-1.383366	-1.580150	0.000000
N	-2.573189	-1.493566	0.000000
C	0.002845	-1.693951	0.000000
N	1.190764	-1.811095	0.000000
C	1.382396	1.623708	0.000000
C	0.000000	1.675455	0.000000
C	2.616316	1.566959	0.000000
H	3.685989	1.517225	0.000000
C	-1.235427	1.716304	0.000000
H	-2.305595	1.765452	0.000000

Tz/Tz

N	0.850330	-1.353190	1.198482
C	1.353946	-1.005975	0.000000
N	0.850330	-1.353190	-1.198482
C	-0.249243	-2.127167	-1.128067
N	-0.846117	-2.551023	0.000000
C	-0.249243	-2.127167	1.128067
H	2.250018	-0.385068	0.000000
H	-0.694242	-2.441657	-2.072074
H	-0.694242	-2.441657	2.072074

N	0.262672	2.175871	1.199399
C	0.744699	2.550363	0.000000
N	0.262672	2.175871	-1.199399
C	-0.800105	1.354622	-1.129453
N	-1.380139	0.906607	0.000000
C	-0.800105	1.354622	1.129453
H	1.599336	3.226856	0.000000
H	-1.229407	1.019556	-2.073363
H	-1.229407	1.019556	2.073363

Bz/Tz

C	-2.081902	1.625544	0.000000
C	-1.379620	1.615231	1.216715
C	0.025611	1.592334	1.217341
C	0.727415	1.579430	0.000000
C	0.025611	1.592334	-1.217341
C	-1.379620	1.615231	-1.216715
H	-3.171530	1.641508	0.000000
H	-1.925060	1.627641	2.160472
H	0.572313	1.582802	2.160365
H	1.817218	1.565443	0.000000
H	0.572313	1.582802	-2.160365
H	-1.925060	1.627641	-2.160472
N	-0.707486	-1.600571	0.000000
C	0.025611	-1.594167	-1.127298
N	1.369439	-1.605811	-1.198632
C	1.979752	-1.618456	0.000000
N	1.369439	-1.605811	1.198632
C	0.025611	-1.594167	1.127298
H	-0.520159	-1.587030	-2.070512
H	3.069569	-1.648315	0.000000
H	-0.520159	-1.587030	2.070512