PBE1PBE/CC-PVDZ energies and geometries for N18C6H6 isomers

Isomer T1 -- PBE1PBE/CC-PVDZ = -1215.854262

N	0.000000	-0.842668	3.604701
N	0.729772	0.421334	3.604701
N	-0.729772	0.421334	3.604701
C	0.000000	-1.305413	2.206935
C	1.130521	0.652706	2.206935
C	-1.130521	0.652706	2.206935
N	0.000000	1.414382	1.659093
N	1.224891	-0.707191	1.659093
N	-1.224891	-0.707191	1.659093
N	0.000000	1.386093	0.197583
N	-1.200392	0.693046	-0.197583
N	-1.200392	-0.693046	0.197583
N	0.000000	-1.386093	-0.197583
N	1.200392	-0.693046	0.197583
N	1.200392	0.693046	-0.197583
N	0.000000	-1.414382	-1.659093
N	1.224891	0.707191	-1.659093
N	-1.224891	0.707191	-1.659093
C	0.000000	1.305413	-2.206935
C	1.130521	-0.652706	-2.206935
C	-1.130521	-0.652706	-2.206935
N	0.000000	0.842668	-3.604701
N	0.729772	-0.421334	-3.604701
N	-0.729772	-0.421334	-3.604701
H	0.000000	-2.396468	2.152688
H	2.075402	1.198234	2.152688
H	-2.075402	1.198234	2.152688
H	0.000000	2.396468	-2.152688
H	2.075402	-1.198234	-2.152688
H	-2.075402	-1.198234	-2.152688

Isomer T2 -- PBE1PBE/CC-PVDZ = -1215.881553

N	0.000000	-0.842022	3.650192
N	0.729212	0.421011	3.650192
N	-0.729212	0.421011	3.650192
C	0.000000	-1.299917	2.248372
C	1.125761	0.649958	2.248372
C	-1.125761	0.649958	2.248372
N	0.000000	1.395993	1.684491
N	1.208966	-0.697997	1.684491
N	-1.208966	-0.697997	1.684491
C	0.000000	1.384103	0.226884
N	-1.218676	0.703603	-0.245470
C	-1.198668	-0.692051	0.226884
N	0.000000	-1.407206	-0.245470
C	1.198668	-0.692051	0.226884
N	1.218676	0.703603	-0.245470
N	0.000000	-1.407960	-1.708493
N	1.219329	0.703980	-1.708493
N	-1.219329	0.703980	-1.708493
N	0.000000	1.323674	-2.223873
N	1.146336	-0.661837	-2.223873

N	-1.146336	-0.661837	-2.223873
N	0.000000	0.866874	-3.566693
N	0.750734	-0.433437	-3.566693
N	-0.750734	-0.433437	-3.566693
H	0.000000	-2.392172	2.191983
H	2.071682	1.196086	2.191983
H	-2.071682	1.196086	2.191983
H	0.000000	2.404739	-0.174592
H	2.082565	-1.202370	-0.174592
H	-2.082565	-1.202370	-0.174592

Isomer T3 -- PBE1PBE/CC-PVDZ = -1215.905243

N	0.000000	-0.869722	3.604348
N	0.753202	0.434861	3.604348
N	-0.753202	0.434861	3.604348
N	0.000000	-1.339946	2.253302
N	1.160428	0.669973	2.253302
N	-1.160428	0.669973	2.253302
C	0.000000	1.379371	1.687188
C	1.194570	-0.689685	1.687188
C	-1.194570	-0.689685	1.687188
N	0.000000	1.357066	0.216991
N	-1.175253	0.678533	-0.216991
N	-1.175253	-0.678533	0.216991
N	0.000000	-1.357066	-0.216991
N	1.175253	-0.678533	0.216991
N	1.175253	0.678533	-0.216991
C	0.000000	-1.379371	-1.687188
C	1.194570	0.689685	-1.687188
C	-1.194570	0.689685	-1.687188
N	0.000000	1.339946	-2.253302
N	1.160428	-0.669973	-2.253302
N	-1.160428	-0.669973	-2.253302
N	0.000000	0.869722	-3.604348
N	0.753202	-0.434861	-3.604348
N	-0.753202	-0.434861	-3.604348
H	0.000000	-2.414942	-2.049346
H	2.091401	1.207471	-2.049346
H	-2.091401	1.207471	-2.049346
H	0.000000	2.414942	2.049346
H	2.091401	-1.207471	2.049346
H	-2.091401	-1.207471	2.049346

Isomer T4 -- PBE1PBE/CC-PVDZ = -1215.913484

N	0.000000	0.870706	-3.599949
N	0.754054	-0.435353	-3.599949
N	-0.754054	-0.435353	-3.599949
N	0.000000	1.338016	-2.250450
N	1.158756	-0.669008	-2.250450
N	-1.158756	-0.669008	-2.250450
C	0.000000	-1.388684	-1.681908
C	1.202635	0.694342	-1.681908
C	-1.202635	0.694342	-1.681908
N	0.000000	-1.395516	-0.221033
C	-1.186333	-0.684930	0.260830

N	-1.208552	0.697758	-0.221033
C	0.000000	1.369860	0.260830
N	1.208552	0.697758	-0.221033
C	1.186333	-0.684930	0.260830
N	0.000000	1.373438	1.734044
N	1.189432	-0.686719	1.734044
N	-1.189432	-0.686719	1.734044
N	0.000000	-1.319564	2.257064
N	1.142776	0.659782	2.257064
N	-1.142776	0.659782	2.257064
N	0.000000	-0.862460	3.609774
N	0.746912	0.431230	3.609774
N	-0.746912	0.431230	3.609774
H	0.000000	2.406447	-0.095909
H	2.084044	-1.203224	-0.095909
H	-2.084044	-1.203224	-0.095909
H	0.000000	-2.411587	-2.083761
H	2.088496	1.205793	-2.083761
H	-2.088496	1.205793	-2.083761

Isomer H1 -- PBE1PBE/CC-PVDZ = -1215.756080

N	0.000000	1.457100	-1.612468
N	1.261886	0.728550	-1.612468
N	1.261886	-0.728550	-1.612468
N	0.000000	-1.457100	-1.612468
N	-1.261886	-0.728550	-1.612468
N	-1.261886	0.728550	-1.612468
C	0.000000	2.314292	-0.383556
C	2.004235	1.157146	-0.383556
C	2.004235	-1.157146	-0.383556
C	0.000000	-2.314292	-0.383556
C	-2.004235	-1.157146	-0.383556
C	-2.004235	1.157146	-0.383556
N	2.325568	0.000000	0.421755
N	1.162784	2.014001	0.421755
N	-1.162784	2.014001	0.421755
N	-2.325568	0.000000	0.421755
N	-1.162784	-2.014001	0.421755
N	1.162784	-2.014001	0.421755
N	1.496859	0.000000	1.619857
N	0.748429	1.296318	1.619857
N	-0.748429	1.296318	1.619857
N	-1.496859	0.000000	1.619857
N	-0.748429	-1.296318	1.619857
N	0.748429	-1.296318	1.619857
H	0.000000	3.364929	-0.702676
H	2.914114	1.682465	-0.702676
H	2.914114	-1.682465	-0.702676
H	0.000000	-3.364929	-0.702676
H	-2.914114	-1.682465	-0.702676
H	-2.914114	1.682465	-0.702676

Isomer H2 -- PBE1PBE/CC-PVDZ = -1215.828431

C	-0.377402	1.406946	1.588284
N	-1.377581	0.367594	1.540221

C	-1.029750	-1.030313	1.588284
N	0.370445	-1.376817	1.540221
C	1.407152	-0.376633	1.588284
N	1.007136	1.009223	1.540221
N	-0.607044	2.272251	0.397850
N	-2.278320	0.608182	0.418735
N	-1.664305	-1.661841	0.397850
N	0.612459	-2.277174	0.418735
N	2.271350	-0.610410	0.397850
N	1.665861	1.668992	0.418735
N	-2.271350	-0.610410	-0.397850
N	-1.665861	1.668992	-0.418735
N	0.607044	2.272251	-0.397850
N	2.278320	0.608182	-0.418735
N	1.664305	-1.661841	-0.397850
N	-0.612459	-2.277174	-0.418735
C	-1.407152	-0.376633	-1.588284
N	-1.007136	1.009223	-1.540221
C	0.377402	1.406946	-1.588284
N	1.377581	0.367594	-1.540221
C	1.029750	-1.030313	-1.588284
N	-0.370445	-1.376817	-1.540221
H	-0.545176	2.028459	2.479123
H	-1.484109	-1.486366	2.479123
H	2.029286	-0.542093	2.479123
H	-2.029286	-0.542093	-2.479123
H	0.545176	2.028459	-2.479123
H	1.484109	-1.486366	-2.479123

Isomer H3 -- PBE1PBE/CC-PVDZ = -1215.802352

C	1.257257	0.725605	1.597316
N	0.000299	1.418811	1.527278
C	-1.257020	0.726014	1.597316
N	-1.228876	-0.709147	1.527278
C	-0.000236	-1.451618	1.597316
N	1.228577	-0.709664	1.527278
N	2.036464	1.175501	0.395159
C	0.000000	2.312089	0.384054
N	-2.036245	1.175879	0.395159
C	-2.002328	-1.156045	0.384054
N	-0.000218	-2.351380	0.395159
C	2.002328	-1.156045	0.384054
N	-1.196632	2.024282	-0.423523
N	1.196968	2.024219	-0.423461
N	2.351396	0.024173	-0.423523
N	1.154541	-2.048714	-0.423461
N	-1.154764	-2.048455	-0.423523
N	-2.351509	0.024495	-0.423461
N	-0.763265	1.280106	-1.612998
N	0.762690	1.279637	-1.611687
N	1.490237	0.020954	-1.612998
N	0.726853	-1.300327	-1.611687
N	-0.726972	-1.301060	-1.612998
N	-1.489543	0.020690	-1.611687
H	1.824545	1.053080	2.482098
H	-1.824267	1.053562	2.482098

H	-0.000278	-2.106643	2.482098
H	-2.919600	-1.685941	0.674310
H	-0.000268	3.371418	0.674310
H	2.919868	-1.685477	0.674310