

Electronic Supplementary Information for

Spectroscopic and *Ab-Initio* Investigation of 2,6-Difluorophenylacetylene-Amine Complexes: Coexistence of C–H⋯N and Lone-pair⋯ π Complexes and Intermolecular Columbic Decay

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Additional Computational Methods

The interaction between DFPHA and TMA was analysed by the topographical study of electron density using the atoms in molecules (AIM)¹ approach using AIM2000 package.² Further, the analysis of the stabilization energies of various structures of DFPHA-TMA complex was carried out using Symmetry Adapted Perturbation Theory (SAPT).³ The simplest of SAPT approach. i.e. SAPT0 with cc-pVTZ basis set along with the cc-pVTZ-JKFIT basis for the Hartree-Fock and cc-pVTZ-RI basis for the SAPT procedure.⁴ The density fitting approach was used to reduce the computational expense. The main advantage of SAPT calculations is that it allows for the separation of interaction energy (E_{SAPT0}) into physically well-defined components, such as those arising from the electrostatic (E_{elec}), induction (E_{ind}) dispersion (E_{disp}) and exchange (E_{exch}) as given in equation (1)

$$E_{\text{SAPT0}} = E_{\text{elec}}^{(10)} + E_{\text{exch}}^{(10)} + E_{\text{ind}}^{(20)} + E_{\text{exch-ind}}^{(20)} + E_{\text{disp}}^{(20)} + E_{\text{exch-disp}}^{(20)} \quad (1)$$

The perturbative method SAPT0 treats the monomers at the Hartree–Fock level and then dissociates the overall intermolecular interaction energy into the different components using second-order perturbation theory. It has been found that the SAPT0 calculations with reasonable basis sets provide good estimates of stabilization energies.⁴ Further, the charge transfer component is given by the equations (2) and (3).⁵

$$E_{\text{Ct}}^{(20)} = E_{\text{Ind}}^{(20)}(\text{dimer}) - E_{\text{Ind}}^{(20)}(\text{monomer}) \quad (2)$$

$$E_{\text{Exch-Ct}}^{(20)} = E_{\text{Exch-Ind}}^{(20)}(\text{dimer}) - E_{\text{Exch-Ind}}^{(20)}(\text{monomer}) \quad (3)$$

In the present analysis the exchange-induction and exchange-dispersion terms will be included to the parent induction and dispersion terms. Even in the case of charge transfer component the difference in the exchange induction term between the dimer and monomer basis is added to the parent charge transfer term. SAPT calculations were carried out using PSI4 *ab-Initio* package.⁶

The stabilization energies of various structures of DFPHA-TMA complex were calculated at MP2/CBS and CCSD(T)/CBS method using extrapolations method proposed by Helgaker co-workers⁷ and are listed in Table S2. Three sets of MP2/CBS and CCSD(T)/CBS extrapolations were carried out. (i) With MP2/aug-cc-pVDZ, MP2/aug-cc-pVTZ (aVTZ) and CCSD(T)/aug-cc-pVDZ energies (Ref. 8) for the geometries obtained at MP2/cc-pVDZ level. (ii) With MP2/cc-pVDZ, MP2/cc-pVTZ and CCSD(T)/cc-pVDZ energies for the geometries

obtained at MP2/cc-pVTZ level. (iii) With MP2/cc-pVDZ (0.25,15), MP2/cc-pVTZ and CCSD(T)/cc-pVDZ (0.25,15) energies for the geometries obtained at MP2/cc-pVTZ level. However, the extrapolations with cc-pVDZ (0.25,0.15) have not benchmarked with molecules containing fluorine (Ref. 9), hence the confidence level on these values is low. Since the intermolecular structures calculated at MP2/cc-pVDZ and MP2/cc-pVTZ are almost identical the best estimates for the stabilization energies are from set 1.

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TABLE S1. ZPE and BSSE corrected energies (kJ mol⁻¹) for the low energy structures of DFPHA-TMA complex calculated at various levels of theory. The ZPE was calculated at MP2/cc-pVDZ level.

Structure	MP2	MP2	MP2	ω B97X-D	B2PLYP-D	B2PLYP-D3
	cc-pVDZ	cc-pVTZ //cc-pVDZ	cc-pVTZ	cc-pVTZ	cc-pVTZ	cc-pVTZ
S ₁	-12.1	-14.8	-14.5	-17.4	-15.5	-15.1
S ₂	-7.9	-10.9	-11.8	-13.9	-12.8	-12.0
S ₃	-7.6	-12.5	-12.7	-15.5	-14.6	-13.1
S ₄	-4.4	-15.4	-15.8	-17.9	-14.9	-14.2
S ₅	-4.1	-16.2	-16.6	-18.8	-15.5	-14.7
S ₆	-2.8	-10.6	-10.6	-13.7	-9.3	-9.00
S ₇	-4.0	-11.0	-11.1	-13.2	-10.5	-9.85
S ₈	-2.8	-7.4	-9.3	-9.7	-8.7	-8.2

TABLE S2. ZPE and BSSE corrected CBS extrapolated stabilization energies (kJ mol⁻¹) for the low energy structures of DFPHA-TMA complex.

Structure	MP2/CBS ^a	MP2/CBS ^b	MP2/CBS ^c	CCSDT/CBS ^a	CCSDT/CBS ^b	CCSDT/CBS ^c
S1	-19.1	-16.9	-16.4	-17.2	-14.8	-14.5
S2	-13.7	-13.9	-12.6	-12.9	-12.3	-11.5
S3	-16.8	-15.2	-13.7	-15.3	-13.5	-12.9
S4	-22.1	-20.5	-16.8	-15.7	-15.1	-11.9
S5	-22.9	-21.7	-18.0	-15.9	-16.3	-12.8
S6	-15.1	-14.0	-11.3	-11.4	-10.43	-8.5
S7	-15.2	-14.3	-11.8	-11.7	-10.93	-9.0
S8	-10.2	-11.8	-9.9	-7.9	-9.15	-7.6

^a aug-cc-pVNZ (N=D,T) basis with MP2/cc-pVDZ optimized geometries.

^b cc-pVNZ (N=D,T) basis with MP2/cc-pVDZ optimized geometries

^c cc-pVNZ(0.25,0.15) (C,N,F and H) (N=D,T) basis with MP2/cc-pVTZ optimized geometry.

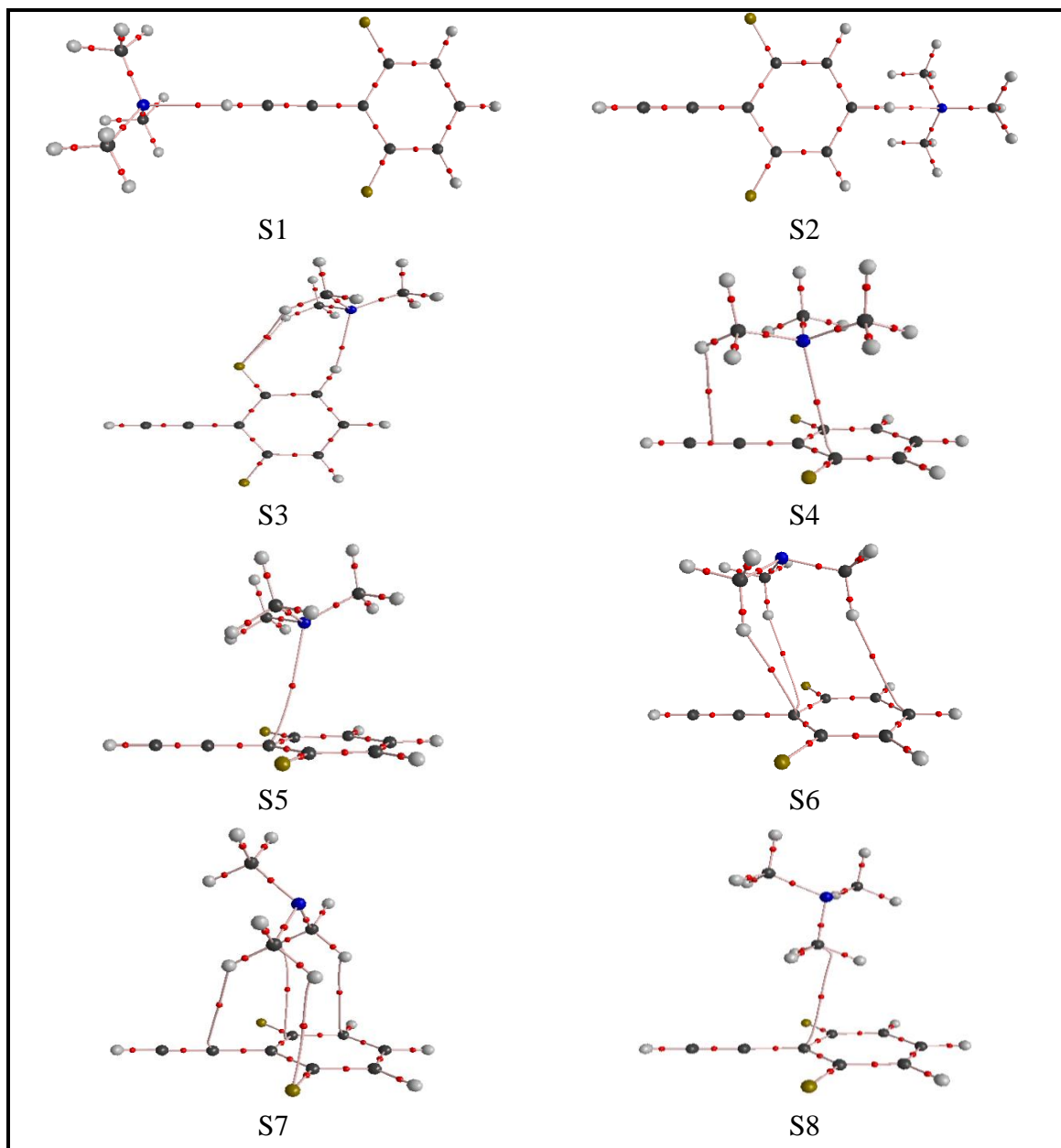


Fig S1. Molecular graphs of various structures of DFPHA-TMA complex calculated for B2PLYPD3/cc-pVTZ level.

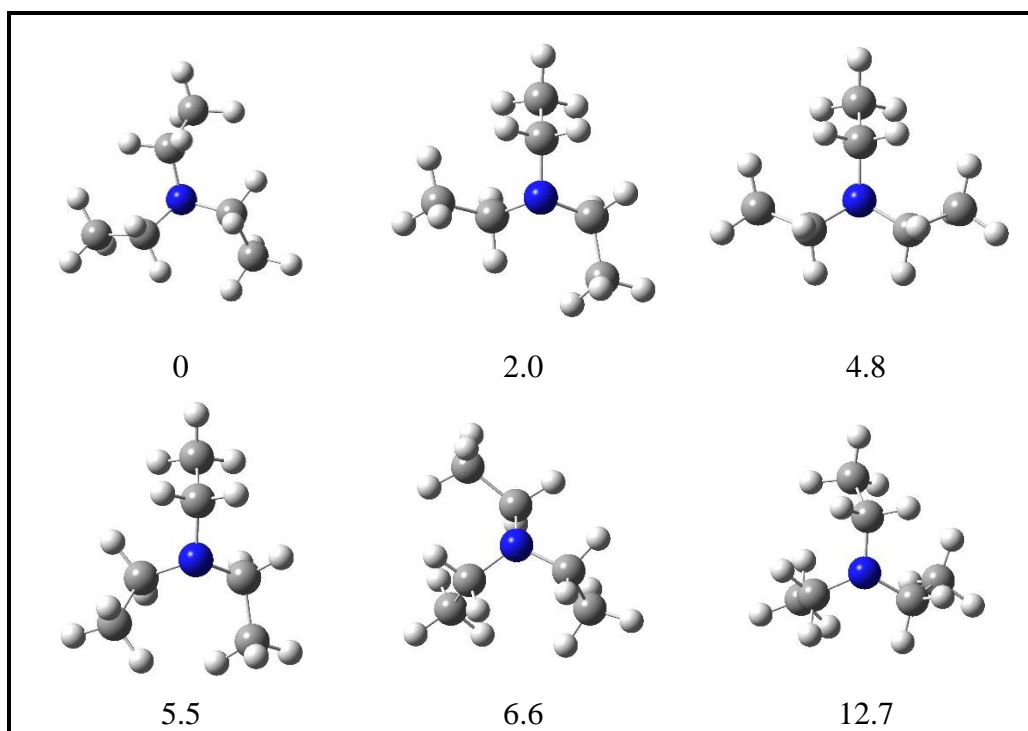


Fig S2. Various conformation of TEA optimized at B3LYP/cc-pVTZ level. Relative energies (kJ mol^{-1}) are given against each structure. Since the experiments were carried out under jet-cooled conditions only the lowest energy structure was considered for calculation of DFPHA-TEA complex.

Optimized coordinates of various structures of DFPHA-TEA complex calculated at various levels of theory viz. MP2/cc-pVDZ, MP2/cc-pVTZ, ω B97X-D/cc-pVTZ, B2PLYP-D/cc-pVTZ and B2PLYP-D3/cc-pVTZ

S1-MP2/cc-pVDZ

C	-1.72361400	0.00042400	-0.00016800
C	-2.46537700	-1.19968100	-0.00005400
C	-3.86176500	-1.22047000	0.00015200
C	-4.55853100	-0.00109900	0.00025700
C	-3.86307400	1.21901800	0.00015600
C	-2.46666300	1.19973300	-0.00005100
C	-0.29096500	0.00117400	-0.00039100
C	0.94532300	0.00177100	-0.00056700
F	-1.79084700	-2.36394000	-0.00014900

F	-1.79338700	2.36471100	-0.00014000
H	-4.37988600	-2.18277500	0.00022800
H	-5.65258500	-0.00168600	0.00041700
H	-4.38222800	2.18076600	0.00023600
H	2.03719200	0.00219400	-0.00077400
N	4.13728500	0.00042000	-0.00003200
C	4.60767300	1.33553700	-0.35764500
H	4.22713100	1.60687100	-1.35555600
H	4.22698200	2.06938800	0.37091100
H	5.71937400	1.40111500	-0.37515800
C	4.60386000	-0.97836500	-0.97775000
H	4.22031100	-1.97702400	-0.71347600
H	4.22335000	-0.71305500	-1.97729700
H	5.71536600	-1.02983400	-1.02665300
C	4.60372300	-0.35848500	1.33609100
H	4.22311600	0.37098000	2.06909800
H	4.22023500	-1.35556900	1.60635300
H	5.71522000	-0.37859400	1.40431900

S1-MP2/cc-pVTZ

C	-1.70276000	0.00127900	-0.00073700
C	-2.44051100	-1.18790400	0.00008500
C	-3.82439900	-1.21157200	0.00164100
C	-4.51617700	-0.00328400	0.00242900
C	-3.82831900	1.20724000	0.00166200
C	-2.44435900	1.18806600	0.00010900
C	-0.28396200	0.00354200	-0.00237100
C	0.93496300	0.00536000	-0.00364000
F	-1.76992500	-2.34591100	-0.00065500
F	-1.77753600	2.34823100	-0.00061800
H	-4.33559900	-2.16247400	0.00221300
H	-5.59652800	-0.00503400	0.00364000

H	-4.34259800	2.15648000	0.00224800
H	2.01265100	0.00683100	-0.00485700
N	4.11521500	0.00226900	-0.00177300
C	4.58832100	1.32987000	-0.35641400
H	4.21776000	1.59893700	-1.34403400
H	4.21376300	2.05631000	0.36268300
H	5.68720100	1.38695700	-0.36918700
C	4.57785600	-0.97408000	-0.97378000
H	4.19536300	-1.95951000	-0.71347800
H	4.20744600	-0.70996000	-1.96280100
H	5.67623300	-1.02657500	-1.01578400
C	4.57288600	-0.35677000	1.33001900
H	4.19864300	0.36599000	2.05299900
H	4.19056400	-1.34085500	1.59563200
H	5.67102500	-0.37990900	1.39712600

S1- ω B97X-D/cc-pVTZ

C	-1.68846600	0.00042700	-0.00056400
C	-2.42638500	-1.18290400	0.00151700
C	-3.80527800	-1.20507900	0.00248900
C	-4.49039500	-0.00099700	0.00136900
C	-3.80649700	1.20377800	-0.00070600
C	-2.42758200	1.18301200	-0.00162700
C	-0.26599500	0.00112300	-0.00153600
C	0.93253500	0.00147500	-0.00235600
F	-1.76457700	-2.33800300	0.00260800
F	-1.76695400	2.33877700	-0.00358900
H	-4.31903100	-2.15463800	0.00410400
H	-5.57104400	-0.00154300	0.00211000
H	-4.32121500	2.15281600	-0.00161100
H	2.01052000	0.00174900	-0.00290400
N	4.13641300	0.00026800	-0.00068000

C	4.57013200	1.33593900	-0.35868300
H	4.18429000	1.59798800	-1.34384800
H	4.18132200	2.05600000	0.36132700
H	5.66809600	1.42929800	-0.38190500
C	4.56763100	-0.97943800	-0.97765600
H	4.17702500	-1.96196600	-0.71277300
H	4.18182900	-0.71405800	-1.96195300
H	5.66541700	-1.05095900	-1.04498700
C	4.56420200	-0.35782800	1.33684500
H	4.17564600	0.36454500	2.05469400
H	4.17384000	-1.34129400	1.59861500
H	5.66174200	-0.38496300	1.43405600

S1-B2PLYP-D/cc-pVTZ

C	-1.68644000	0.00058300	-0.00021500
C	-2.42936200	-1.18578200	-0.00030500
C	-3.81183900	-1.20943400	0.00000500
C	-4.50138900	-0.00139700	0.00044000
C	-3.81353800	1.20760800	0.00056400
C	-2.43102700	1.18590400	0.00023800
C	-0.26728300	0.00155900	-0.00056000
C	0.94132800	0.00232600	-0.00081000
F	-1.76368500	-2.34821000	-0.00071300
F	-1.76698800	2.34926100	0.00037000
H	-4.32278400	-2.15957300	-0.00009300
H	-5.58104800	-0.00215600	0.00068700
H	-4.32581700	2.15702800	0.00090600
H	2.01802700	0.00279700	-0.00102900
N	4.11837800	0.00057200	-0.00018400
C	4.57097900	1.33538500	-0.35774700
H	4.19115300	1.59888600	-1.34393800
H	4.19066800	2.05669400	0.36429600

H	5.66971500	1.40830600	-0.37701600
C	4.56632300	-0.97837700	-0.97762200
H	4.18245500	-1.96259300	-0.71258000
H	4.18668000	-0.71197600	-1.96311500
H	5.66480000	-1.03613300	-1.03178100
C	4.56582200	-0.35836100	1.33596400
H	4.18577600	0.36508200	2.05602900
H	4.18205100	-1.34333100	1.59834600
H	5.66426500	-0.38114100	1.41221800

S1-B2PLYP-D3/cc-pVTZ

C	-1.69412500	0.00068100	-0.00026800
C	-2.43575200	-1.18549200	-0.00044700
C	-3.81758600	-1.20923000	-0.00000600
C	-4.50667900	-0.00165700	0.00065300
C	-3.81959300	1.20705900	0.00086400
C	-2.43771900	1.18562200	0.00040300
C	-0.27556000	0.00183300	-0.00077300
C	0.93264200	0.00278500	-0.00117300
F	-1.76808700	-2.34654500	-0.00107500
F	-1.77198600	2.34777600	0.00061200
H	-4.32914500	-2.15882900	-0.00018000
H	-5.58616700	-0.00255300	0.00100300
H	-4.33272800	2.15580700	0.00137400
H	2.00800400	0.00347300	-0.00142200
N	4.13244400	0.00075800	-0.00031900
C	4.57991100	1.33715300	-0.35843800
H	4.19779000	1.60071100	-1.34305000
H	4.19704700	2.05789000	0.36190100
H	5.67730100	1.41936900	-0.38004200
C	4.57440000	-0.97984200	-0.97883300
H	4.18732400	-1.96235500	-0.71465600

H	4.19249200	-0.71426400	-1.96299500
H	5.67144100	-1.04526800	-1.03981000
C	4.57353100	-0.35866600	1.33781500
H	4.19095600	0.36356900	2.05682600
H	4.18655000	-1.34168700	1.60025300
H	5.67051200	-0.38457300	1.42414100

S2-MP2/cc-pVDZ

C	2.46790400	0.02071700	-0.00845100
C	1.85913300	-1.25122900	-0.03854300
C	0.47368500	-1.41583100	-0.08820500
C	-0.35209700	-0.27899100	-0.10975200
C	0.21694500	1.00602700	-0.08085300
C	1.60592600	1.13660900	-0.03133100
C	3.89258500	0.17154000	0.04279100
C	5.11852700	0.30146000	0.08683300
F	2.65546600	-2.33658100	-0.01781900
F	2.15595700	2.36533000	-0.00369600
H	0.06000800	-2.42750800	-0.10976800
H	-1.44404200	-0.38549700	-0.14627200
H	-0.40043600	1.90810300	-0.09742300
H	6.18768200	0.41454900	0.12520800
N	-3.72103000	-0.06165600	-0.01192300
C	-3.72109800	1.38456000	0.17953100
H	-3.08320500	1.64395600	1.04058600
H	-3.31339000	1.87740100	-0.71848200
H	-4.74217200	1.79005700	0.36659800
C	-4.23322600	-0.72472600	1.18233400
H	-4.21220200	-1.81710700	1.03823200
H	-3.59590700	-0.47575000	2.04639400
H	-5.27950900	-0.42363700	1.42029600
C	-4.53046300	-0.41547600	-1.17276400

H	-4.11949800	0.06916000	-2.07312800
H	-4.50575200	-1.50678400	-1.32360700
H	-5.59410500	-0.10205700	-1.06108700

S2-MP2/cc-pVTZ

C	2.32389500	0.03695800	0.09959300
C	1.60996400	-1.15721200	0.24720300
C	0.27272200	-1.27299100	-0.08941700
C	-0.39593100	-0.16127600	-0.59793100
C	0.27579900	1.04856200	-0.76119800
C	1.61299800	1.12715700	-0.41383900
C	3.69541100	0.13705400	0.45180800
C	4.87045500	0.22279400	0.75346400
F	2.25767700	-2.22198700	0.73589000
F	2.26365500	2.28678200	-0.56880400
H	-0.22455200	-2.22212100	0.04592500
H	-1.44672600	-0.23346500	-0.85222400
H	-0.21905000	1.92452000	-1.15397200
H	5.89609400	0.29753500	1.01641600
N	-3.68752400	-0.04512000	-0.21118100
C	-3.58301500	1.32706500	0.25448600
H	-2.62310200	1.47417500	0.74813300
H	-3.64594500	2.00853600	-0.59263400
H	-4.38183000	1.58558200	0.96669300
C	-3.58572600	-0.95695900	0.91525900
H	-3.65060300	-1.98530800	0.56275800
H	-2.62583000	-0.81982200	1.41180200
H	-4.38465200	-0.79355100	1.65497400
C	-4.94765600	-0.24447800	-0.90555100
H	-5.00675700	0.42801600	-1.75940800
H	-5.00897100	-1.26895600	-1.26817800
H	-5.81511600	-0.05485100	-0.25436800

S2- ω B97X-D/cc-pVTZ

C	2.31535300	0.04083200	0.10317900
C	1.59965800	-1.14575100	0.26051300
C	0.26823800	-1.26334900	-0.07698300
C	-0.39123500	-0.16016900	-0.59641900
C	0.27623600	1.04225900	-0.77047400
C	1.60753800	1.12187200	-0.42153700
C	3.68890600	0.14296100	0.45866200
C	4.84437900	0.22887300	0.75778300
F	2.23664200	-2.20296200	0.75959200
F	2.25221400	2.27488600	-0.58722600
H	-0.23333500	-2.20853800	0.06820100
H	-1.44223400	-0.23329800	-0.85069200
H	-0.21893400	1.91392100	-1.17178700
H	5.86980600	0.30494700	1.02292500
N	-3.70162700	-0.04034900	-0.18296900
C	-3.58601600	1.33505900	0.25634900
H	-2.62743000	1.48389700	0.75509000
H	-3.63151100	2.00390500	-0.60349800
H	-4.38622700	1.62340200	0.95802400
C	-3.58443500	-0.95724600	0.93224100
H	-3.62921100	-1.98567900	0.57294200
H	-2.62570700	-0.81064800	1.43137000
H	-4.38425100	-0.81960400	1.67869300
C	-4.92496800	-0.26015200	-0.92579700
H	-4.95986400	0.40579400	-1.78800100
H	-4.95943100	-1.28776500	-1.28762200
H	-5.82686700	-0.08045900	-0.31686200

S2-B2PLYP-D/cc-pVTZ

C	2.33406100	0.04574700	0.10425700
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C	1.59601900	-1.12652000	0.30472500
C	0.25597200	-1.23338000	-0.01669900
C	-0.39537700	-0.13240100	-0.56563800
C	0.29465200	1.05663400	-0.78388100
C	1.63404800	1.12409200	-0.44917300
C	3.70968100	0.13587800	0.44271200
C	4.87865100	0.21241400	0.73028400
F	2.22442100	-2.18520800	0.83311900
F	2.29974600	2.26772700	-0.65845000
H	-0.25636500	-2.16600400	0.16237400
H	-1.44724800	-0.19827000	-0.81101200
H	-0.18696200	1.92424400	-1.20773800
H	5.90642500	0.27963500	0.98281200
N	-3.70167000	-0.05236000	-0.21037100
C	-3.60686800	1.32620900	0.24055600
H	-2.64563500	1.48653400	0.72808700
H	-3.68032500	1.99815400	-0.61390400
H	-4.40500800	1.58588300	0.95441800
C	-3.57692100	-0.96431400	0.91459700
H	-3.62602000	-1.99353500	0.56049800
H	-2.61666400	-0.81016300	1.40595300
H	-4.37490100	-0.81662400	1.65991300
C	-4.94759200	-0.27862500	-0.92327800
H	-5.00678300	0.39009700	-1.78092700
H	-4.98432500	-1.30647000	-1.28167900
H	-5.82932600	-0.10273600	-0.28585600

S2-B2PLYP-D3/cc-pVTZ

C	2.37569300	0.03709400	0.08260800
C	1.64536300	-1.14133700	0.26917700
C	0.29560600	-1.23836500	-0.00907600
C	-0.37339700	-0.12039400	-0.49763000

C	0.30876400	1.07540100	-0.69957700
C	1.65829600	1.13260500	-0.40943500
C	3.76169300	0.11669000	0.37567000
C	4.93979900	0.18433600	0.62464800
F	2.29307600	-2.21552900	0.73968000
F	2.31869600	2.28209600	-0.60260200
H	-0.21104700	-2.17643300	0.15603300
H	-1.43323400	-0.17794600	-0.70924100
H	-0.18749700	1.95584100	-1.07703500
H	5.97537900	0.24374800	0.84326300
N	-3.71549800	-0.03486200	-0.16626100
C	-3.68902900	1.33744900	0.31178100
H	-2.78810000	1.50429000	0.90036800
H	-3.67859800	2.02197200	-0.53488800
H	-4.56009800	1.58100500	0.93976700
C	-3.68736500	-0.96941300	0.94650700
H	-3.67448300	-1.99070300	0.56921000
H	-2.78712800	-0.80947500	1.53808300
H	-4.55893900	-0.85938300	1.61036600
C	-4.86932100	-0.27003000	-1.01771500
H	-4.84580000	0.41178500	-1.86591000
H	-4.84494200	-1.29004000	-1.39698700
H	-5.82220300	-0.12376300	-0.48510500

S3-MP2/cc-pVDZ

C	-2.01439200	0.32236400	-0.00008000
C	-0.60455600	0.28735600	-0.00014700
C	0.12879100	-0.90039200	-0.00009900
C	-0.57977700	-2.11417600	-0.00000600
C	-1.98467200	-2.13551200	0.00004800
C	-2.67667900	-0.92301900	0.00000600
C	-2.73900000	1.55924000	-0.00016600

C	-3.36483100	2.62237000	0.00032600
F	0.05142900	1.47071100	-0.00026200
F	-4.02236600	-0.92815100	0.00005000
H	1.22648100	-0.85720700	-0.00014100
H	-0.02673400	-3.05852000	0.00001700
H	-2.55017300	-3.07088000	0.00012700
H	-3.91016500	3.54976200	0.00041400
N	3.33071500	-0.06711300	0.00004600
C	3.27256400	0.76991000	-1.19483600
C	4.55076000	-0.86564000	0.00011700
C	3.27243300	0.76990900	1.19492200
H	3.29742400	0.13365000	-2.09467900
H	2.33090600	1.34103500	-1.19429800
H	4.12296000	1.48786500	-1.25022600
H	4.57349800	-1.50974900	0.89419000
H	4.57370600	-1.50958500	-0.89406800
H	5.47088000	-0.23662600	0.00027900
H	2.33074300	1.34098100	1.19432700
H	3.29727700	0.13365000	2.09476600
H	4.12278700	1.48791000	1.25036500

S3-MP2/cc-pVTZ

C	-2.02851200	0.32673300	0.00008200
C	-0.62967000	0.30619000	0.00003800
C	0.11154300	-0.86200600	0.00002800
C	-0.57499500	-2.07455600	0.00005600
C	-1.96742800	-2.11281600	0.00003800
C	-2.66627700	-0.91857500	0.00005900
C	-2.76100000	1.54273100	0.00005400
C	-3.38795700	2.58495000	0.00000300
F	0.01142300	1.48694000	0.00000500
F	-4.00454700	-0.94224300	0.00001200

H	1.19591200	-0.80922000	-0.00000600
H	-0.01709400	-3.00011400	0.00003100
H	-2.51448800	-3.04367300	0.00000600
H	-3.93636800	3.49374800	-0.00001400
N	3.33611400	-0.07596800	0.00001600
C	3.28482600	0.75685400	-1.19031600
C	4.54817200	-0.87593100	0.00001500
C	3.28474500	0.75672900	1.19043200
H	3.30302100	0.12764400	-2.07887300
H	2.36282100	1.33539700	-1.19203000
H	4.13457000	1.45486700	-1.24218600
H	4.56952500	-1.51122300	0.88384200
H	4.56958200	-1.51113600	-0.88387300
H	5.45599000	-0.25261000	0.00007500
H	2.36274400	1.33527800	1.19213800
H	3.30286800	0.12742400	2.07892300
H	4.13448900	1.45473000	1.24243900

S3- ω B97X-D/cc-pVTZ

C	-2.04118200	0.32674700	0.00002600
C	-0.64682000	0.32218900	-0.00001700
C	0.10454300	-0.83256000	-0.00002200
C	-0.56381500	-2.04698100	0.00001300
C	-1.94860100	-2.10414100	0.00005200
C	-2.65937300	-0.92308300	0.00006500
C	-2.79083300	1.53575900	0.00002700
C	-3.42156100	2.55270400	0.00002800
F	-0.01955600	1.50178100	-0.00005300
F	-3.99014200	-0.96828500	0.00008400
H	1.18796800	-0.76860400	-0.00005400
H	0.00638500	-2.96522800	0.00000500
H	-2.48261300	-3.04254800	0.00007400

H	-3.98213600	3.45455000	0.00004200
N	3.36392600	-0.04547500	0.00002400
C	3.30824800	0.77077500	-1.19609900
C	4.52567100	-0.90916100	0.00003300
C	3.30814100	0.77065400	1.19622500
H	3.30124500	0.13230800	-2.07980300
H	2.39399300	1.36385700	-1.19513200
H	4.16617700	1.45884100	-1.27574500
H	4.51349000	-1.54782800	0.88346800
H	4.51356600	-1.54774200	-0.88346500
H	5.47227900	-0.34293200	0.00010100
H	2.39388900	1.36374000	1.19523300
H	3.30105400	0.13209800	2.07986400
H	4.16606500	1.45870900	1.27601900

S3-B2PLYP-D/cc-pVTZ

C	2.00852100	0.32896400	0.00008100
C	0.61011300	0.27802400	-0.00001300
C	-0.10951300	-0.90120900	-0.00026700
C	0.59822100	-2.09984900	-0.00044000
C	1.98977600	-2.11302500	-0.00035700
C	2.66498400	-0.90701800	-0.00010200
C	2.71871200	1.55814000	0.00034700
C	3.32138700	2.60307300	0.00057400
F	-0.05838700	1.44558200	0.00015700
F	4.00468100	-0.91162400	-0.00002200
H	-1.19269600	-0.86578300	-0.00033800
H	0.05761200	-3.03474200	-0.00064100
H	2.55392100	-3.03269200	-0.00048800
H	3.85240000	3.52103000	0.00077600
N	-3.33532900	-0.07084600	-0.00011300
C	-3.24223600	0.75246700	1.19529600

C	-4.56583800	-0.84305800	-0.00026900
C	-3.24248600	0.75337200	-1.19491400
H	-3.28183000	0.11890800	2.08079300
H	-2.29733900	1.29290900	1.19322700
H	-4.06307300	1.48499400	1.25690600
H	-4.60245800	-1.47716900	-0.88531900
H	-4.60227100	-1.47783300	0.88431200
H	-5.46026200	-0.19885000	0.00006600
H	-2.29757400	1.29378800	-1.19265800
H	-3.28230700	0.12048700	-2.08088500
H	-4.06331700	1.48596800	-1.25578600

S3-B2PLYP-D3/cc-pVTZ

C	2.03345300	0.31909500	0.00008700
C	0.63519600	0.28715200	0.00004100
C	-0.09873200	-0.88265600	-0.00025300
C	0.59319500	-2.08968500	-0.00051800
C	1.98389600	-2.12101300	-0.00049500
C	2.67412700	-0.92428300	-0.00019200
C	2.75919300	1.53841900	0.00038300
C	3.37533100	2.57520300	0.00064600
F	-0.01599400	1.46365600	0.00029600
F	4.01359000	-0.94400700	-0.00018100
H	-1.18121800	-0.83349100	-0.00027000
H	0.04064600	-3.01738100	-0.00075400
H	2.53538800	-3.04808600	-0.00070800
H	3.91799900	3.48585400	0.00086800
N	-3.34392500	-0.03894900	-0.00002300
C	-3.29080500	0.78463100	1.19740200
C	-4.52492000	-0.88482800	-0.00022800
C	-3.29088500	0.78532200	-1.19697600
H	-3.29141600	0.14850500	2.08111400

H	-2.37578900	1.37338600	1.19624400
H	-4.14655700	1.47388600	1.26901600
H	-4.52236600	-1.52130600	-0.88354300
H	-4.52230700	-1.52181600	0.88272000
H	-5.45962600	-0.30200300	-0.00002800
H	-2.37586600	1.37407200	-1.19554100
H	-3.29156100	0.14970600	-2.08105400
H	-4.14663900	1.47462300	-1.26813100

S4-MP2/cc-pVDZ

C	-0.86372500	0.59724800	0.48715500
C	-0.49977500	-0.58458300	1.16323300
C	-1.09459400	-1.81574600	0.88259000
C	-2.08991000	-1.88265500	-0.10815100
C	-2.48015700	-0.72984400	-0.80808300
C	-1.86216500	0.48486700	-0.49956100
C	-0.23265900	1.85042500	0.77318900
C	0.28864300	2.94134600	1.02086200
F	0.44470400	-0.51295300	2.11462500
F	-2.21539900	1.59457500	-1.17638700
H	-0.77779000	-2.69932700	1.44289500
H	-2.56613000	-2.84154100	-0.33434200
H	-3.24937800	-0.75555000	-1.58414600
H	0.74722200	3.88950500	1.24088900
N	1.92152000	-0.27687600	-0.51901200
C	2.43827300	-1.60272100	-0.21438200
C	2.98319400	0.71517100	-0.42804800
C	1.31535600	-0.25877100	-1.84207700
H	2.85212600	-1.61189100	0.80710000
H	1.61714500	-2.33770300	-0.26203500
H	3.23727000	-1.92820900	-0.92178500
H	2.57035900	1.71459200	-0.63835500

H	3.39438300	0.72122800	0.59475600
H	3.81791900	0.51826700	-1.14178400
H	0.49458600	-0.99484900	-1.87996400
H	0.89142500	0.74005900	-2.04046900
H	2.04159300	-0.49947600	-2.65418500

S4-MP2/cc-pVTZ

C	-0.87899800	0.61228500	0.49519100
C	-0.52250700	-0.54169900	1.19987700
C	-1.08191500	-1.77820300	0.93086000
C	-2.03903700	-1.88053000	-0.07704900
C	-2.42631600	-0.75854300	-0.80438700
C	-1.84107400	0.46052100	-0.50641100
C	-0.27125500	1.86573300	0.76111000
C	0.24290100	2.94549600	0.98646400
F	0.39028200	-0.43677700	2.16844100
F	-2.19189700	1.54276800	-1.21375400
H	-0.76915600	-2.63491200	1.50911000
H	-2.48648300	-2.83976600	-0.29455200
H	-3.16438100	-0.81282200	-1.59052700
H	0.68839800	3.88753500	1.18913500
N	1.91975000	-0.29325900	-0.52686700
C	2.40691100	-1.63514300	-0.27912900
C	2.99384200	0.67130000	-0.39530200
C	1.31338600	-0.20677500	-1.84029600
H	2.82206800	-1.69361300	0.72605700
H	1.58106000	-2.34251500	-0.35290900
H	3.18670000	-1.93920100	-0.99632200
H	2.60172900	1.67421900	-0.55483300
H	3.40752500	0.62142700	0.61076800
H	3.80794700	0.49301100	-1.11675800
H	0.49035800	-0.91828900	-1.90950800

H	0.91460300	0.79586000	-1.99424800
H	2.02959700	-0.42352000	-2.64963400

S4- ω B97X-D/cc-pVTZ

C	-0.92502500	0.67371000	0.49769100
C	-0.52296400	-0.44282200	1.22832700
C	-1.03202700	-1.70269400	0.99839600
C	-1.97828900	-1.86773200	-0.00061200
C	-2.41015600	-0.79026600	-0.75638800
C	-1.87686200	0.45457800	-0.49435900
C	-0.35986300	1.95857500	0.72250300
C	0.12040500	3.03984300	0.90371000
F	0.38457400	-0.27931500	2.18365300
F	-2.27378000	1.49335800	-1.22746700
H	-0.68075300	-2.53128800	1.59454500
H	-2.38556700	-2.85034900	-0.19202800
H	-3.14510700	-0.89832700	-1.53963200
H	0.54133500	4.00038900	1.07015200
N	1.95328400	-0.38148900	-0.57740300
C	2.39954700	-1.74600700	-0.42359900
C	2.99951000	0.56947800	-0.27829300
C	1.36456600	-0.14904200	-1.87605500
H	2.76952100	-1.90138400	0.59039100
H	1.56369000	-2.42763100	-0.58858700
H	3.20542900	-2.01553300	-1.12844500
H	2.59991900	1.58189700	-0.33561800
H	3.36461900	0.40834500	0.73618000
H	3.85616400	0.49223700	-0.97057900
H	0.53085000	-0.83583200	-2.03037000
H	0.97792800	0.86951300	-1.92911400
H	2.08308400	-0.28762500	-2.702468

S4-B2PLYP-D/cc-pVTZ

C	-0.89397000	0.63495100	0.48594000
C	-0.50879600	-0.50776100	1.19451200
C	-1.05252300	-1.75472600	0.95259500
C	-2.02345400	-1.88319300	-0.03651900
C	-2.43981800	-0.77866400	-0.77141800
C	-1.86891500	0.45111100	-0.49735400
C	-0.30015100	1.90057100	0.72467700
C	0.20392200	2.97881500	0.92218600
F	0.42196500	-0.38255700	2.14469600
F	-2.25195800	1.51660300	-1.21519900
H	-0.71304500	-2.59867100	1.53254300
H	-2.45841200	-2.85138200	-0.23513200
H	-3.18825300	-0.85357300	-1.54468700
H	0.64281400	3.92736500	1.10185600
N	1.93272900	-0.32285000	-0.54530900
C	2.38898000	-1.68161400	-0.33359500
C	3.00167700	0.63225300	-0.32745900
C	1.34328700	-0.16414500	-1.86004300
H	2.77521500	-1.78315700	0.68022600
H	1.55298500	-2.37044500	-0.45563000
H	3.18429400	-1.97505400	-1.03952800
H	2.61293000	1.64289800	-0.44124200
H	3.38601900	0.52421800	0.68616900
H	3.83794200	0.49445700	-1.03386700
H	0.51357300	-0.86163900	-1.97448700
H	0.95780000	0.84946800	-1.96780400
H	2.06719900	-0.34869200	-2.67159900

S4-B2PLYP-D3/cc-pVTZ

C	-0.92940200	0.67702000	0.48360700
C	-0.50507500	-0.42437500	1.23247900

C	-1.01677000	-1.69387700	1.04865300
C	-1.98935000	-1.88909800	0.07374800
C	-2.44198000	-0.82817600	-0.70247100
C	-1.90613200	0.42704700	-0.48280400
C	-0.37400100	1.96815300	0.67038800
C	0.09978600	3.06680000	0.82478700
F	0.43151600	-0.23166800	2.16606500
F	-2.32765900	1.45361800	-1.23444200
H	-0.64870800	-2.50431600	1.65776100
H	-2.39818300	-2.87616300	-0.08192000
H	-3.19408100	-0.95664900	-1.46478200
H	0.51066300	4.03377800	0.96609500
N	1.93591100	-0.38301400	-0.59712600
C	2.35207000	-1.76715200	-0.49480300
C	2.99741700	0.52216300	-0.20029100
C	1.44026700	-0.07328300	-1.92398500
H	2.66166200	-1.98196200	0.52712100
H	1.51688300	-2.42065300	-0.74371400
H	3.19155900	-2.01123400	-1.16652700
H	2.63388800	1.54703100	-0.23759600
H	3.29834700	0.30584900	0.82338800
H	3.88640400	0.44245800	-0.84759700
H	0.61033100	-0.73498100	-2.16858800
H	1.07706100	0.95300700	-1.94941100
H	2.21161300	-0.18573600	-2.70350300

S5-MP2/cc-pVDZ

C	-1.25926000	0.10100600	0.00170500
C	-0.84588400	0.71560500	-1.19589100
C	-0.06983300	1.87466500	-1.21439300
C	0.31778000	2.44895800	0.00668400
C	-0.06529800	1.86645200	1.22529300

C	-0.84138700	0.70752400	1.20185300
C	-2.03120800	-1.10560000	-0.00089300
C	-2.68149200	-2.15491700	-0.00316300
F	-1.20340800	0.14147500	-2.36091800
F	-1.19443900	0.12544500	2.36429800
H	0.21763700	2.30909900	-2.17545100
H	0.92384900	3.36021500	0.00862400
H	0.22579200	2.29438300	2.18817700
H	-3.25992400	-3.06227400	-0.00511500
N	1.72749300	-0.72075300	-0.00399300
C	3.02368500	-0.06101700	-0.00452100
C	1.57009700	-1.53673600	-1.19997000
C	1.57410800	-1.54242700	1.18859800
H	3.11040300	0.58166100	-0.89653800
H	3.11318500	0.57759800	0.89014400
H	3.87777700	-0.77953600	-0.00748600
H	0.57035300	-2.00181000	-1.20149700
H	1.65348000	-0.90046900	-2.09690500
H	2.33431100	-2.34649400	-1.27353500
H	1.66053700	-0.91045200	2.08827400
H	0.57437300	-2.00748800	1.19132600
H	2.33855700	-2.35252200	1.25570600

S5-MP2/cc-pVTZ

C	-1.27340600	0.11151500	0.00225800
C	-0.86523000	0.72633200	-1.18425600
C	-0.09772200	1.87632300	-1.20422900
C	0.28631000	2.44559300	0.00661300
C	-0.09418000	1.86944300	1.21531600
C	-0.86174300	0.71957200	1.19104900
C	-2.02617500	-1.09095100	-0.00006000
C	-2.66077600	-2.12952600	-0.00209000

F	-1.22178900	0.15801500	-2.34399900
F	-1.21488500	0.14464600	2.34857900
H	0.18650700	2.30589700	-2.15330700
H	0.88527500	3.34519700	0.00829500
H	0.19283500	2.29361000	2.16598700
H	-3.22170500	-3.03086800	-0.00383100
N	1.75354200	-0.72863100	-0.00432300
C	3.05253400	-0.08827400	-0.00434300
C	1.58212400	-1.53582600	-1.19668200
C	1.58550000	-1.54260800	1.18389900
H	3.14808700	0.54449800	-0.88608700
H	3.15059000	0.53947700	0.88070900
H	3.88233500	-0.81425900	-0.00758100
H	0.58917200	-1.98467400	-1.19618400
H	1.67271600	-0.90720200	-2.08206600
H	2.32832200	-2.34402900	-1.26758200
H	1.67866800	-0.91904900	2.07259200
H	0.59252400	-1.99140300	1.18369100
H	2.33185400	-2.35122900	1.24804900

S5- ω B97X-D/cc-pVTZ

C	-1.29810600	0.14530000	0.00232100
C	-0.89571900	0.76309800	-1.17897200
C	-0.14087500	1.91523100	-1.19873600
C	0.23582200	2.48233300	0.00721200
C	-0.13766900	1.90809100	1.21077100
C	-0.89256100	0.75607600	1.18618400
C	-2.03434100	-1.07088700	-0.00030500
C	-2.63701600	-2.10524600	-0.00254700
F	-1.24397100	0.19935800	-2.33454600
F	-1.23768300	0.18544700	2.33931000
H	0.14394300	2.34607800	-2.14670900

H	0.83107600	3.38435900	0.00909000
H	0.14970100	2.33329200	2.16052200
H	-3.17999300	-3.01781800	-0.00451300
N	1.80876900	-0.79549600	-0.00469400
C	3.08483100	-0.12063500	-0.00509100
C	1.60994300	-1.57938000	-1.20274400
C	1.61381200	-1.58540300	1.19002700
H	3.16506500	0.51677900	-0.88652400
H	3.16793800	0.51241200	0.87921800
H	3.94017900	-0.81916600	-0.00821800
H	0.61148700	-2.01834900	-1.19583900
H	1.69057200	-0.93924200	-2.08212500
H	2.34462400	-2.39705400	-1.30446800
H	1.69798400	-0.94983400	2.07238100
H	0.61507800	-2.02377000	1.18446200
H	2.34839400	-2.40398500	1.28494600

S5-B2PLYP-D/cc-pVTZ

C	-1.27281300	-0.05247700	0.00052800
C	-0.95628300	0.61737400	-1.18421400
C	-0.37255800	1.86858200	-1.20704600
C	-0.08175500	2.49015500	0.00213600
C	-0.37100500	1.86633000	1.21052400
C	-0.95471600	0.61514600	1.18611000
C	-1.83648600	-1.35415300	-0.00033400
C	-2.30261800	-2.46733600	-0.00108100
F	-1.21503800	0.00106300	-2.34636300
F	-1.21189800	-0.00335800	2.34743400
H	-0.15137500	2.33138300	-2.15609900
H	0.37644700	3.46796000	0.00275100
H	-0.14857500	2.32735200	2.16015100
H	-2.72029300	-3.44219900	-0.00170300

N	1.86859200	-0.52095700	-0.00098800
C	3.10034200	0.24206800	0.00224200
C	1.75820400	-1.33237500	-1.19881600
C	1.75675000	-1.34008700	1.19146800
H	3.13802400	0.88090400	-0.87994600
H	3.13694100	0.87512800	0.88862600
H	3.99651100	-0.40186900	0.00070300
H	0.80662800	-1.86257400	-1.19667400
H	1.79257300	-0.69266100	-2.08045000
H	2.56967400	-2.07544800	-1.27810500
H	1.78992000	-0.70607300	2.07724700
H	0.80523500	-1.87034600	1.18467200
H	2.56820500	-2.08356700	1.26699600

S5-B2PLYP-D3/cc-pVTZ

C	-1.30026500	0.14969700	0.00352700
C	-0.90031200	0.77038200	-1.18210500
C	-0.14943700	1.92859300	-1.20668100
C	0.22895600	2.50275100	0.00121200
C	-0.13957400	1.92459300	1.21021200
C	-0.89030000	0.76626200	1.18788500
C	-2.03857800	-1.06097600	0.00444800
C	-2.65563700	-2.09779700	0.00507600
F	-1.25037300	0.19782800	-2.34244600
F	-1.23038800	0.18957300	2.34914200
H	0.12948300	2.35822700	-2.15589800
H	0.81772700	3.40774900	0.00029600
H	0.14722300	2.35095800	2.15855300
H	-3.20487300	-3.00457600	0.00568000
N	1.79946200	-0.79976600	-0.00311900
C	3.07907100	-0.12026100	0.00369400
C	1.62524100	-1.59089900	-1.20666700

C	1.62243200	-1.60934700	1.18772100
H	3.15930800	0.52003300	-0.87369700
H	3.15719700	0.50626800	0.89116300
H	3.93339600	-0.81758700	-0.00067100
H	0.63541300	-2.04432800	-1.20839700
H	1.70712800	-0.95016200	-2.08354900
H	2.37354000	-2.39536900	-1.29762600
H	1.70040100	-0.98196500	2.07456000
H	0.63334700	-2.06431500	1.17925500
H	2.37169500	-2.41397500	1.26884400

S6-MP2/cc-pVDZ

C	-1.04360100	0.72242500	0.00217100
C	-1.29870100	0.02749300	1.20220500
C	-1.78771500	-1.28007800	1.22098800
C	-2.03718100	-1.92734200	-0.00059200
C	-1.79346500	-1.27535500	-1.22080600
C	-1.30398200	0.03203000	-1.19933700
C	-0.55615400	2.06944300	0.00379500
C	-0.11907700	3.22344900	0.00525500
F	-1.04064100	0.65501900	2.36356400
F	-1.05083800	0.66375800	-2.35947600
H	-1.96306900	-1.77021400	2.18201600
H	-2.42082100	-2.95201100	-0.00167100
H	-1.97355200	-1.76176200	-2.18285400
H	0.24777700	4.23509400	0.00652600
N	2.87404400	-0.68943700	-0.00454000
C	2.63828800	0.10040400	1.19853700
C	1.99448600	-1.85157600	-0.01491700
C	2.63893200	0.12096800	-1.19401200
H	2.85784500	-0.51062400	2.09011100
H	3.31101400	0.97397400	1.20616400

H	1.59157900	0.47125800	1.28138000
H	2.19351100	-2.45977200	-0.91330700
H	2.19241500	-2.47503700	0.87318700
H	0.91454300	-1.57809400	-0.01333200
H	3.31064200	0.99531200	-1.18557100
H	2.86026700	-0.47420000	-2.09581800
H	1.59186500	0.49197300	-1.27156200

S6-MP2/cc-pVTZ

C	-1.04732400	0.72616100	0.00435300
C	-1.29497200	0.02793200	1.19129900
C	-1.76366200	-1.27392900	1.20768600
C	-1.99900000	-1.91673100	-0.00507400
C	-1.76591700	-1.26447300	-1.21321800
C	-1.29721100	0.03723000	-1.18753800
C	-0.56329600	2.05961700	0.00915100
C	-0.13799900	3.19946100	0.01332600
F	-1.05789300	0.65295400	2.34966300
F	-1.06233200	0.67128700	-2.34143400
H	-1.93463300	-1.76176400	2.15556900
H	-2.36412200	-2.93361200	-0.00870000
H	-1.93863700	-1.74489100	-2.16456500
H	0.22534900	4.19706100	0.01698300
N	2.85894300	-0.69682500	-0.00500500
C	2.63651900	0.10003900	1.18850000
C	1.97045700	-1.84460900	-0.00800400
C	2.63348400	0.10855200	-1.19221000
H	2.83288800	-0.50342100	2.07368600
H	3.31804000	0.94944200	1.19441100
H	1.60843800	0.48697700	1.25507400
H	2.15671100	-2.45079200	-0.89374600
H	2.15930400	-2.45743500	0.87260400

H	0.90750800	-1.55645900	-0.00535300
H	3.31434800	0.95849700	-1.19332500
H	2.82846600	-0.48828600	-2.08218300
H	1.60495400	0.49511700	-1.25384600

S6- ω B97X-D/cc-pVTZ

C	-1.07371500	0.71503700	0.00439400
C	-1.32871600	0.02079400	1.18630600
C	-1.81038000	-1.27068300	1.20313700
C	-2.05088300	-1.90608700	-0.00430000
C	-1.81248200	-1.26190900	-1.20749600
C	-1.33072400	0.02939300	-1.18209200
C	-0.56522100	2.04272600	0.00871100
C	-0.12123800	3.15384500	0.01213200
F	-1.08581300	0.63533400	2.34075900
F	-1.08966700	0.65224100	-2.33247300
H	-1.98500500	-1.75831000	2.15020000
H	-2.42557000	-2.91956700	-0.00765500
H	-1.98868000	-1.74265800	-2.15777600
H	0.26733100	4.14215800	0.01517900
N	2.85146100	-0.66881000	-0.00498900
C	2.65893300	0.11698300	1.19506900
C	2.00771100	-1.84326600	-0.00933400
C	2.65669800	0.12746700	-1.19776800
H	2.86939200	-0.49275200	2.07441100
H	3.34594400	0.96370000	1.19703300
H	1.63507100	0.51375300	1.29006400
H	2.21470500	-2.44545100	-0.89477200
H	2.21541500	-2.45248900	0.87110300
H	0.93190800	-1.59905000	-0.00797200
H	3.34474300	0.97334700	-1.19432200
H	2.86409600	-0.47497400	-2.08284300

H	1.63309800	0.52632600	-1.28660200
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S6-B2PLYP-D/cc-pVTZ

C	-1.03739000	0.72690700	0.00307200
C	-1.28765300	0.02783400	1.18888800
C	-1.76724400	-1.26806400	1.20964900
C	-2.01155400	-1.90882500	-0.00058100
C	-1.77555000	-1.26164100	-1.20904500
C	-1.29575200	0.03412600	-1.18473600
C	-0.54223200	2.05617600	0.00500600
C	-0.11199400	3.18303000	0.00742200
F	-1.03807000	0.64661800	2.34936400
F	-1.05415200	0.65906000	-2.34356700
H	-1.93647800	-1.75318500	2.15814100
H	-2.38401700	-2.92215600	-0.00199700
H	-1.95143700	-1.74170300	-2.15890600
H	0.26085700	4.17597700	0.00941000
N	2.83313300	-0.68282300	-0.00612000
C	2.62515700	0.10999300	1.19370800
C	1.96757500	-1.84879100	-0.00885500
C	2.62173300	0.11799700	-1.20001100
H	2.83300000	-0.49799800	2.07405000
H	3.30703600	0.95991800	1.19330600
H	1.59856000	0.49789200	1.27708000
H	2.16692000	-2.45121700	-0.89510500
H	2.16906600	-2.45698800	0.87296200
H	0.89850700	-1.58457900	-0.00670000
H	3.30333700	0.96813300	-1.19572000
H	2.82737000	-0.48398100	-2.08498700
H	1.59477000	0.50610900	-1.27795800

S6-B2PLYP-D3/cc-pVTZ

C	-1.09468800	0.73679600	0.00500500
C	-1.34712300	0.03753400	1.18954300
C	-1.82111400	-1.25996700	1.20801700
C	-2.05793000	-1.90103900	-0.00293400
C	-1.82119300	-1.25266800	-1.21001000
C	-1.34708900	0.04464900	-1.18370600
C	-0.60311100	2.06692000	0.00902100
C	-0.17436600	3.19410700	0.01256200
F	-1.10671100	0.65934600	2.35020200
F	-1.10641000	0.67334700	-2.34060400
H	-1.99301500	-1.74629600	2.15518800
H	-2.42628200	-2.91568400	-0.00598300
H	-1.99305600	-1.73329800	-2.16009100
H	0.19662500	4.18729200	0.01562600
N	2.88533300	-0.68879300	-0.00581900
C	2.67746000	0.09878200	1.19664200
C	2.03736200	-1.86664800	-0.01124800
C	2.67655800	0.11055600	-1.20034000
H	2.89387300	-0.50844300	2.07454700
H	3.35358700	0.95236500	1.19764300
H	1.64984400	0.48104600	1.28930100
H	2.24592200	-2.46595300	-0.89657200
H	2.24625800	-2.47432300	0.86826900
H	0.96372400	-1.62238800	-0.00991400
H	3.35352700	0.96345800	-1.19402200
H	2.89119700	-0.48836000	-2.08436100
H	1.64923000	0.49476100	-1.28785600

S7-MP2/cc-pVDZ

C	-1.24585200	0.62522300	-0.09822700
C	-1.27694700	0.16378600	1.23379400
C	-1.60547100	-1.15227900	1.56535200

C	-1.92335800	-2.05040900	0.53296900
C	-1.90359600	-1.63566800	-0.80896700
C	-1.56794200	-0.31217800	-1.10126900
C	-0.90952500	1.98069300	-0.41715500
C	-0.61511700	3.14689800	-0.69202200
F	-0.95432400	1.02973700	2.21279400
F	-1.53479400	0.09310600	-2.38270600
H	-1.60796100	-1.45303700	2.61609300
H	-2.18335800	-3.08491100	0.77636900
H	-2.14216300	-2.31815500	-1.62865400
H	-0.36503000	4.16574500	-0.93154000
N	2.88001800	-0.57778600	0.31604800
C	4.07972900	-0.45452500	-0.50032300
C	2.42911700	0.74474600	0.73219700
C	1.83035400	-1.24171100	-0.44513500
H	4.87936800	0.03187000	0.08235800
H	4.43128600	-1.45531100	-0.80105400
H	3.91041400	0.14635300	-1.42557300
H	1.53130700	0.65726900	1.36461600
H	3.21981700	1.23681800	1.32270000
H	2.17614900	1.40382400	-0.13118300
H	2.17130100	-2.24492600	-0.75162300
H	0.93159000	-1.35720100	0.18104200
H	1.54086800	-0.67687300	-1.36396900

S7-MP2/cc-pVTZ

C	-1.16849300	0.64156500	-0.20753200
C	-1.17400300	0.27770700	1.14358500
C	-1.50933500	-0.99448000	1.57396100
C	-1.86131100	-1.95097700	0.62479000
C	-1.87280500	-1.63626700	-0.73195800
C	-1.52794500	-0.35390500	-1.12132600

C	-0.80572100	1.94716600	-0.62919000
C	-0.48464100	3.06529700	-0.98617400
F	-0.83117100	1.20248100	2.04802300
F	-1.52151700	-0.04417800	-2.42223500
H	-1.49366700	-1.21675300	2.63042000
H	-2.12665700	-2.94842400	0.94440800
H	-2.13949800	-2.36310400	-1.48441300
H	-0.21153600	4.04246200	-1.29903400
N	2.86773400	-0.69570000	0.27376300
C	3.94699800	-0.22159900	-0.57246400
C	2.34030500	0.40305400	1.06446900
C	1.81558300	-1.26260700	-0.55033800
H	4.74570700	0.18888200	0.04307100
H	4.35114700	-1.04981100	-1.15252900
H	3.61428700	0.56054400	-1.27426100
H	1.56804100	0.03689900	1.73974000
H	3.13881000	0.83693900	1.66451200
H	1.90369000	1.19949300	0.43945500
H	2.20365700	-2.11452000	-1.10758600
H	0.99480900	-1.60564000	0.07832300
H	1.41341100	-0.53342400	-1.27254600

S7- ω B97X-D/cc-pVTZ

C	-1.17447200	0.61734200	-0.22713300
C	-1.20268700	0.31049200	1.13190700
C	-1.57611300	-0.92803700	1.60931500
C	-1.94554200	-1.90679500	0.70103400
C	-1.94013900	-1.65165800	-0.66082600
C	-1.55624700	-0.40201200	-1.09792700
C	-0.75136600	1.88931900	-0.70054600
C	-0.37855000	2.95429200	-1.09899900
F	-0.84173300	1.25364900	1.99783500

F	-1.53071000	-0.15445300	-2.40448900
H	-1.57304800	-1.10812600	2.67369800
H	-2.24021600	-2.88265200	1.05946500
H	-2.22098300	-2.40235200	-1.38390100
H	-0.05280100	3.90120200	-1.45264400
N	2.89224200	-0.67767400	0.19965300
C	3.96083000	-0.08228100	-0.57197300
C	2.33538400	0.26746100	1.14366100
C	1.86817000	-1.22369300	-0.66376200
H	4.74728300	0.27403100	0.09394500
H	4.39405800	-0.82558900	-1.24205400
H	3.61754100	0.77031300	-1.18407800
H	1.58643900	-0.22643800	1.76319000
H	3.12131500	0.64270900	1.79964500
H	1.85690200	1.13189300	0.65235900
H	2.29354300	-1.99893400	-1.30215200
H	1.07541500	-1.67255900	-0.06354100
H	1.41136500	-0.45835100	-1.31474700

S7-B2PLYP-D/cc-pVTZ

C	-1.18825500	0.65164500	-0.13622700
C	-1.17864500	0.22633900	1.19597200
C	-1.53361600	-1.05370400	1.57879500
C	-1.92232200	-1.96014500	0.59785800
C	-1.95002600	-1.58899400	-0.74254800
C	-1.58424400	-0.30018900	-1.08181600
C	-0.80046100	1.96420700	-0.50924300
C	-0.46308400	3.07763300	-0.82783400
F	-0.79437900	1.09995700	2.13497300
F	-1.59183300	0.05789900	-2.37136500
H	-1.50108800	-1.32045400	2.62355400
H	-2.20201900	-2.96410300	0.87968000

H	-2.24247900	-2.27672600	-1.52047800
H	-0.16988600	4.05783700	-1.10749800
N	2.84620700	-0.71708200	0.19418800
C	3.94029400	-0.19368400	-0.60304900
C	2.34003500	0.30205200	1.09786900
C	1.78462300	-1.21059500	-0.66472200
H	4.74477700	0.14298400	0.05009800
H	4.32871300	-0.97601400	-1.25462100
H	3.62914500	0.65645400	-1.23388300
H	1.55880700	-0.11909700	1.72835700
H	3.14654800	0.65464200	1.74017100
H	1.91902200	1.16890100	0.56299800
H	2.16578100	-2.01305700	-1.29625700
H	0.97019900	-1.60373000	-0.05756100
H	1.37564300	-0.42272000	-1.31902600

S7-B2PLYP-D3/cc-pVTZ

C	-1.23213000	0.62454400	-0.18821000
C	-1.24677700	0.25683000	1.16054800
C	-1.58650300	-1.01218200	1.58903000
C	-1.93285800	-1.96660600	0.63892400
C	-1.93516500	-1.65350700	-0.71589600
C	-1.58672300	-0.37337200	-1.10131100
C	-0.86355800	1.92817600	-0.60727600
C	-0.54223400	3.03438300	-0.96434100
F	-0.90390400	1.17884600	2.06874900
F	-1.57288100	-0.06766300	-2.40413300
H	-1.57538300	-1.23434100	2.64440400
H	-2.20020500	-2.96297800	0.95669800
H	-2.19608700	-2.37955800	-1.46955800
H	-0.26349800	4.00804400	-1.27801600
N	2.93170500	-0.65164200	0.23580100

C	4.02345200	-0.17942600	-0.59525000
C	2.39703700	0.42622800	1.04969300
C	1.89020300	-1.25404400	-0.57609700
H	4.81439900	0.23005400	0.03119800
H	4.43636800	-1.00821300	-1.16847500
H	3.70789400	0.60354400	-1.30467700
H	1.62049300	0.04187200	1.70826100
H	3.18888300	0.84614200	1.66815900
H	1.96258800	1.23989400	0.44765400
H	2.29768600	-2.09755700	-1.13188400
H	1.08844300	-1.62022100	0.06289600
H	1.45463400	-0.54614900	-1.29995700

S8-MP2/cc-pVDZ

C	1.62806300	0.45214100	-0.01672400
C	1.91198200	-0.62226300	-0.88482800
C	1.76184400	-1.95592700	-0.49745600
C	1.32088400	-2.23891100	0.80581100
C	1.03010900	-1.20003900	1.70522400
C	1.18685300	0.12045900	1.28059400
C	1.76868100	1.81527000	-0.43454200
C	1.88023200	2.99026000	-0.79331200
F	2.33732500	-0.34006200	-2.12842500
F	0.88559900	1.12538700	2.12344200
H	1.99465600	-2.74786500	-1.21385700
H	1.20081500	-3.27917000	1.12280000
H	0.68111800	-1.39537500	2.72235100
H	1.98044000	4.01434800	-1.10789500
N	-3.13045900	0.25626000	-0.55531300
C	-4.10626900	0.91634400	0.30032100
H	-3.67694100	1.84827500	0.70310700
H	-5.00402300	1.17362700	-0.28557100

H	-4.42376800	0.28019000	1.16091300
C	-1.93199800	-0.05717400	0.20916800
H	-1.18619100	-0.54014200	-0.44334800
H	-1.49096900	0.86933900	0.61224500
H	-2.13618400	-0.74413300	1.06614400
C	-3.69786300	-0.96480700	-1.10895400
H	-4.59218100	-0.72429600	-1.70711200
H	-2.96069500	-1.45103000	-1.76892100
H	-3.99429400	-1.69763600	-0.32061500

S8-MP2/cc-pVTZ

C	1.40357600	0.38313600	0.32099800
C	1.68768100	-0.33347400	-0.84598500
C	1.69644800	-1.71661100	-0.88954000
C	1.41047000	-2.42525500	0.27465000
C	1.12101300	-1.75652600	1.46161500
C	1.12292100	-0.37275900	1.46379800
C	1.37538000	1.80151500	0.33814600
C	1.34004000	3.01734900	0.35009500
F	1.94536100	0.35765100	-1.96157100
F	0.83139300	0.27988900	2.59414300
H	1.91894500	-2.21429200	-1.82140600
H	1.41230600	-3.50555600	0.25662500
H	0.89365000	-2.28575500	2.37479200
H	1.31532700	4.07864000	0.36233900
N	-3.12782400	-0.20412400	-0.74279300
C	-3.82963300	1.06118100	-0.84910800
H	-3.38038300	1.66548900	-1.63538400
H	-4.87327800	0.88433800	-1.10422700
H	-3.79564200	1.63696600	0.09012400
C	-1.73208700	0.03091200	-0.42576300
H	-1.20409100	-0.92009600	-0.35981700

H	-1.26851000	0.62959900	-1.20926000
H	-1.60497500	0.56402500	0.53145100
C	-3.73429700	-1.02210200	0.29022000
H	-4.77743700	-1.21477600	0.04457000
H	-3.21389500	-1.97643000	0.35574200
H	-3.69569100	-0.53986400	1.28079400

S8- ω B97X-D/cc-pVTZ

C	1.44658300	0.38963300	0.32814000
C	1.72463300	-0.32023800	-0.83881100
C	1.72614600	-1.69795500	-0.89122300
C	1.43855200	-2.40712200	0.26368300
C	1.15430900	-1.74996200	1.45002500
C	1.16352500	-0.37149500	1.46112600
C	1.42278500	1.81107600	0.35407000
C	1.38982100	3.00699800	0.37288800
F	1.98596100	0.36859000	-1.94626100
F	0.87797600	0.26728300	2.59228900
H	1.94466600	-2.19205100	-1.82574800
H	1.43344800	-3.48739400	0.23828000
H	0.92364600	-2.28517100	2.35867300
H	1.36512900	4.06853400	0.39090400
N	-3.16259100	-0.19493200	-0.70862400
C	-3.87710200	1.05344000	-0.86050100
H	-3.42561600	1.64455500	-1.65755300
H	-4.91581500	0.85771000	-1.12840000
H	-3.86976000	1.66146900	0.06127800
C	-1.76401700	0.03228300	-0.42041000
H	-1.23738700	-0.92102100	-0.35972200
H	-1.30718500	0.62264400	-1.21527900
H	-1.60745800	0.57014600	0.53129900
C	-3.77425800	-1.03278900	0.29880300

H	-4.81308000	-1.23437600	0.03575500
H	-3.24747700	-1.98572800	0.35855300
H	-3.75866700	-0.57105900	1.30201300

S8-B2PLYP-D/cc-pVTZ

C	1.41402300	0.39208600	0.34736600
C	1.70023000	-0.32966400	-0.81608600
C	1.70380600	-1.71109300	-0.86124000
C	1.40881500	-2.41738700	0.30027300
C	1.11477000	-1.74894200	1.48445200
C	1.12252500	-0.36686800	1.48551100
C	1.39212200	1.81055000	0.36469000
C	1.36382700	3.01637000	0.37682000
F	1.96681000	0.35662600	-1.93392800
F	0.82411100	0.28262000	2.61715800
H	1.92824400	-2.20832100	-1.79182000
H	1.40544500	-3.49688600	0.28188800
H	0.87813500	-2.27614200	2.39535800
H	1.34345400	4.07672000	0.38900400
N	-3.11739500	-0.19903500	-0.75735000
C	-3.82809800	1.05903300	-0.89560100
H	-3.35449700	1.66613400	-1.66625300
H	-4.86020500	0.86992600	-1.18919100
H	-3.83671800	1.63942900	0.04280000
C	-1.72855600	0.03602800	-0.40825900
H	-1.19973100	-0.91367000	-0.33727600
H	-1.24969400	0.64214000	-1.17646900
H	-1.62197700	0.56233600	0.55554200
C	-3.75577500	-1.03933900	0.23878300
H	-4.78784900	-1.23617500	-0.04979500
H	-3.22891800	-1.99049900	0.30989300
H	-3.76013900	-0.57290700	1.23897600

S8-B2PLYP-D3/cc-pVTZ

C	1.45236900	0.39492900	0.36279200
C	1.75659800	-0.32915200	-0.79402500
C	1.78272000	-1.71011000	-0.82945800
C	1.49350600	-2.41274200	0.33508600
C	1.18333800	-1.74173600	1.51299100
C	1.16862100	-0.36023300	1.50482100
C	1.41048200	1.81252700	0.37112300
C	1.36482600	3.01762400	0.37559700
F	2.02078500	0.35540000	-1.91334000
F	0.85810200	0.29357700	2.63056000
H	2.02081000	-2.21060600	-1.75465200
H	1.50804000	-3.49206800	0.32411500
H	0.95210600	-2.26720300	2.42604400
H	1.32943300	4.07723000	0.38112900
N	-3.17401500	-0.19467900	-0.77240300
C	-3.87333400	1.06900800	-0.91368900
H	-3.39134100	1.67286300	-1.68075900
H	-4.90382800	0.88964200	-1.21645800
H	-3.88703500	1.65208800	0.02210200
C	-1.78214200	0.02066800	-0.42365500
H	-1.26514800	-0.93562600	-0.36176100
H	-1.29619900	0.62382200	-1.18886500
H	-1.66259100	0.53834900	0.54240700
C	-3.82618400	-1.04156500	0.20858200
H	-4.85690500	-1.22750800	-0.08940000
H	-3.31011200	-1.99851500	0.27035900
H	-3.83613500	-0.59291300	1.21600500

Optimized coordinates of various structures of DFPHA-TEA complex calculated at MP2/cc-pVDZ level of theory.

S9

C	-2.43997900	-0.00899300	-0.00072900
C	-3.19153000	-1.20302400	-0.00053500
C	-4.58796400	-1.21152100	0.00015100
C	-5.27393000	0.01398600	0.00072700
C	-4.56823200	1.22824900	0.00063400
C	-3.17212400	1.19708400	-0.00008900
C	-1.00787700	-0.01979200	-0.00141900
C	0.22894700	-0.02678500	-0.00199400
F	-2.52648500	-2.37247700	-0.00101900
F	-2.48815400	2.35565700	-0.00012700
H	-5.11461200	-2.16917900	0.00024800
H	-6.36793800	0.02283000	0.00127100
H	-5.07929600	2.19431200	0.00110000
H	1.32003700	-0.02789900	-0.00199300
N	3.46074100	0.00409100	0.00051000
C	3.95752300	-0.96700800	0.99185300
H	5.03555300	-0.78097700	1.20731800
H	3.89710300	-1.97113800	0.54198300
C	3.91605100	1.36073600	0.35432600
H	4.99606500	1.48197000	0.10516900
H	3.83297100	1.47128300	1.44757600
C	3.94895100	-0.35532700	-1.34301100
H	3.85494000	0.53418600	-1.98661600
H	5.03492900	-0.60502500	-1.30481100
C	3.15781500	-1.49763400	-1.97767300
H	3.55613600	-1.71804800	-2.98249200
H	3.21716800	-2.42590700	-1.38716700

H	2.09534000	-1.22334400	-2.07717600
C	3.14432800	-0.96658700	2.28501600
H	3.55053300	-1.71651300	2.98466500
H	3.17023900	0.00985700	2.79474200
H	2.09124100	-1.21715900	2.07959000
C	3.08643300	2.45961900	-0.30747500
H	3.46380100	3.45021800	-0.00215300
H	3.13233800	2.41289900	-1.40731900
H	2.02954500	2.38236100	-0.00589700

S10

C	-3.11087700	0.00501600	0.00106300
C	-2.45291100	1.25285000	-0.00906400
C	-1.06139600	1.36418200	-0.02076300
C	-0.28058600	0.19591400	-0.02295800
C	-0.89891200	-1.06660400	-0.01400600
C	-2.29278900	-1.14385200	-0.00186200
C	-4.54108700	-0.09042300	0.01309400
C	-5.77187900	-0.17311400	0.02333800
F	-3.20682800	2.36813200	-0.00734200
F	-2.89087200	-2.34988300	0.00675400
H	-0.60949800	2.35978300	-0.02949100
H	0.81520300	0.25468400	-0.02786700
H	-0.31388100	-1.99059500	-0.01905500
H	-6.84527200	-0.24483200	0.03238200
N	3.13357200	-0.03846100	0.00126200
C	3.48470400	-1.04933900	1.01222000
H	4.57539700	-1.01108300	1.24132700
H	3.29317200	-2.04462600	0.57879600
C	3.77699900	1.24584900	0.32186100

H	4.85192300	1.22935400	0.02625500
H	3.75677700	1.37471000	1.41630100
C	3.54811200	-0.49104800	-1.33676500
H	3.58781000	0.39153000	-1.99618600
H	4.58211200	-0.90767600	-1.30509900
C	2.58130900	-1.50570200	-1.94458000
H	2.93105900	-1.81069800	-2.94543200
H	2.49735700	-2.41840100	-1.33221200
H	1.57577700	-1.06660700	-2.04533200
C	2.66308400	-0.91137500	2.29255100
H	2.95307200	-1.69189900	3.01627800
H	2.81438900	0.06538700	2.77995600
H	1.58854200	-1.01881400	2.07308400
C	3.06410100	2.43468400	-0.31945600
H	3.58420900	3.37426300	-0.06694700
H	3.03124700	2.35636800	-1.41815500
H	2.02766100	2.50192100	0.04982100

S11

C	2.63726400	-0.22571800	-0.01464400
C	1.22933700	-0.30267600	-0.03409800
C	0.40603600	0.82481900	-0.06283400
C	1.01488300	2.09126900	-0.06785300
C	2.41382100	2.22303600	-0.04843000
C	3.19866500	1.06860700	-0.02158800
C	3.45760900	-1.40090600	0.01196600
C	4.16394200	-2.41216500	0.03338100
F	0.66477200	-1.53030500	-0.03247600
F	4.53966200	1.18019700	-0.00257500
H	-0.68259200	0.68534200	-0.06972300

H	0.38890500	2.98905800	-0.08689700
H	2.90451000	3.19975000	-0.05240200
H	4.78015800	-3.29383200	0.05318000
N	-2.80150000	-0.18047200	0.02887600
C	-2.75222800	-1.41900600	-0.76654500
H	-3.78005500	-1.82836400	-0.90995300
H	-2.19156100	-2.16810300	-0.18460500
C	-3.83441200	0.72790500	-0.49303900
H	-4.84824700	0.40140400	-0.16346100
H	-3.82782600	0.66182000	-1.59282300
C	-3.08625800	-0.50766200	1.43737500
H	-3.48734100	0.39681800	1.92406300
H	-3.88990400	-1.27839400	1.49759400
C	-1.84798300	-0.96499400	2.20629500
H	-2.12690500	-1.25060800	3.23485400
H	-1.36012200	-1.83155200	1.73387400
H	-1.10671500	-0.15176400	2.26077300
C	-2.05566700	-1.24229900	-2.11422800
H	-2.05109000	-2.20084700	-2.66029800
H	-2.55934300	-0.50011900	-2.75425500
H	-1.01203500	-0.92588200	-1.96729100
C	-3.58251500	2.18031400	-0.09280400
H	-4.37670500	2.83329500	-0.49300200
H	-3.56281100	2.31065900	1.00138500
H	-2.61469000	2.52245700	-0.49540400

S12

C	-1.31393800	0.64105100	0.61099200
C	-1.79296000	1.01428900	-0.66158100
C	-2.61839400	0.18722900	-1.42630000

C	-3.00195200	-1.05874100	-0.90283200
C	-2.55259300	-1.47100500	0.36247700
C	-1.72653300	-0.61682500	1.09544000
C	-0.50869600	1.52558000	1.39809800
C	0.17102400	2.29994300	2.07760700
F	-1.43808600	2.21933800	-1.14634300
F	-1.30299300	-0.99959600	2.31577600
H	-2.95689900	0.53225000	-2.40665600
H	-3.65097600	-1.71648000	-1.48868400
H	-2.83736200	-2.43482200	0.79207000
H	0.75770900	2.97499600	2.67602100
N	1.88093100	-0.41137100	-0.40372700
C	2.49651700	-1.29319300	0.60074400
H	3.59486500	-1.38193700	0.41946200
H	2.07821700	-2.30426800	0.46563600
C	2.70784300	0.79315400	-0.56478300
H	3.68555900	0.53978200	-1.04286800
H	2.94020400	1.16981400	0.44483000
C	1.77010800	-1.12994400	-1.68107800
H	1.63323300	-0.38586500	-2.48175800
H	2.71564300	-1.67571000	-1.91523000
C	0.57716500	-2.08326400	-1.70874400
H	0.49018200	-2.56011400	-2.70036800
H	0.66756200	-2.88779800	-0.96061900
H	-0.34839300	-1.52605400	-1.49923800
C	2.22873900	-0.85489900	2.03889200
H	2.70272400	-1.56353600	2.73986500
H	2.63524800	0.14647200	2.25267300
H	1.14732900	-0.83113900	2.23631200
C	2.01571600	1.91128800	-1.34198000

H	2.64465500	2.81791100	-1.32787100
H	1.84663200	1.64987200	-2.39893400
H	1.04477800	2.15058200	-0.88517400

S13

C	-1.75115400	0.49157400	-0.42606900
C	-0.86674000	-0.27070500	-1.21720800
C	-0.89471600	-1.66731700	-1.23060400
C	-1.83892300	-2.33573900	-0.43440500
C	-2.74090100	-1.61617000	0.36732000
C	-2.68315700	-0.22144600	0.35703600
C	-1.72719800	1.92407000	-0.43231500
C	-1.70548900	3.15797200	-0.43172200
F	0.00995700	0.38140800	-2.00004200
F	-3.54180600	0.48098400	1.11796100
H	-0.19068300	-2.20997300	-1.86514200
H	-1.87186300	-3.42950400	-0.43797300
H	-3.48362600	-2.11500900	0.99508000
H	-1.69141100	4.23396100	-0.43740400
N	2.08469000	-0.02766800	0.49827300
C	1.89054800	-0.93311100	1.64007100
H	2.67886300	-0.76608700	2.41323600
H	2.02637800	-1.96575200	1.27585700
C	2.32333700	1.34198700	0.97696600
H	3.33976900	1.43142700	1.43097100
H	1.60145600	1.54637300	1.78447700
C	3.22887400	-0.49144700	-0.30152500
H	3.62397700	0.36506000	-0.87087700
H	4.05783300	-0.83816900	0.35962600
C	2.83703500	-1.58533900	-1.29263400

H	3.72043800	-1.93081100	-1.85662200
H	2.39952700	-2.46126600	-0.78542400
H	2.09481800	-1.18911200	-2.00238800
C	0.50097300	-0.82451100	2.26321300
H	0.39896200	-1.54934600	3.08919200
H	0.30452500	0.17794200	2.67663000
H	-0.26842000	-1.04080500	1.50799100
C	2.13012500	2.39267200	-0.11487400
H	2.25065800	3.40386600	0.31039000
H	2.86458000	2.28827100	-0.92984400
H	1.12234600	2.30614200	-0.54646100

S14

C	-1.67472600	0.72299900	0.01689700
C	-1.87947900	0.00699900	1.21417300
C	-2.27262000	-1.33258300	1.22846000
C	-2.47279500	-1.99252500	0.00464500
C	-2.27425700	-1.32093300	-1.21343200
C	-1.88310900	0.01922800	-1.18741300
C	-1.29107500	2.10301400	0.02175500
C	-0.94365400	3.28731100	0.02069400
F	-1.66587900	0.64689300	2.37833600
F	-1.68084000	0.67274400	-2.34520800
H	-2.41364100	-1.83693100	2.18782600
H	-2.78071800	-3.04245800	-0.00024500
H	-2.41834400	-1.81594300	-2.17723300
H	-0.65720600	4.32467000	0.02175500
N	2.18072800	-0.32059800	-0.01474900
C	1.97506500	0.64493100	1.07531700
H	0.91263800	0.66625400	1.40563300

H	2.19596000	1.65356600	0.68749900
C	1.41859500	-1.55109500	0.23713900
H	0.34834500	-1.42873200	-0.04137300
H	1.43781400	-1.74582900	1.32327100
C	1.81212000	0.26440700	-1.31241300
H	1.62147600	-0.56311300	-2.01699400
H	0.86611800	0.84507900	-1.24550300
C	2.93001900	1.13727700	-1.87846400
H	2.64707800	1.53913400	-2.86641600
H	3.15062300	1.99390400	-1.22032300
H	3.85248300	0.54367700	-1.98369200
C	2.89540500	0.36110000	2.26057100
H	2.74441800	1.10749200	3.05923800
H	2.70607000	-0.63500300	2.69400200
H	3.94731800	0.39358700	1.93392600
C	2.02122400	-2.75618600	-0.48194600
H	1.45068300	-3.67207300	-0.24992700
H	2.01263000	-2.62625200	-1.57675400
H	3.06735400	-2.89723100	-0.16549700

S15

C	-1.79907000	-0.49545400	0.59157800
C	-2.10904300	0.86279300	0.80937200
C	-2.45183000	1.72914800	-0.23029400
C	-2.49349400	1.22965500	-1.54305600
C	-2.19051500	-0.11643500	-1.80726200
C	-1.85185100	-0.95277600	-0.74080600
C	-1.43321100	-1.36382400	1.67014300
C	-1.10095500	-2.11421200	2.59177300
F	-2.04408200	1.33291200	2.06752700

F	-1.54271600	-2.23942900	-0.98345400
H	-2.67867700	2.77360100	-0.00126100
H	-2.76058300	1.89662900	-2.36828900
H	-2.21427100	-0.52723200	-2.81987300
H	-0.82211000	-2.76851700	3.39935600
N	2.31235700	0.25077600	-0.28698300
C	1.81457200	-1.09332100	-0.61580500
H	0.95846600	-1.37742900	0.03737200
H	2.61880600	-1.81798700	-0.40484000
C	1.18836100	1.17231400	-0.07358800
H	0.76431100	1.05704400	0.95134900
H	0.38311900	0.89851200	-0.77481600
C	3.16834100	0.20717200	0.90536800
H	3.22310900	1.22740000	1.32115000
H	2.71648900	-0.43238000	1.70011100
C	4.58593600	-0.25925700	0.58013800
H	5.21693700	-0.24335800	1.48513500
H	4.60036900	-1.28688600	0.18190100
H	5.03209700	0.40501000	-0.17729400
C	1.43058200	-1.21080200	-2.08929900
H	1.05596700	-2.22376200	-2.31335400
H	0.63775500	-0.49422900	-2.35979800
H	2.30793700	-1.00110600	-2.72239600
C	1.57929600	2.62593200	-0.32943300
H	0.70741100	3.28915700	-0.19418900
H	2.37000900	2.96782900	0.35871700
H	1.95481800	2.73532600	-1.35974000

S16

C	1.89755500	0.47401400	0.20695700
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C	1.55192100	-0.04189500	1.47249900
C	1.59020000	-1.40766800	1.76104900
C	1.99596400	-2.30079800	0.75554400
C	2.34938300	-1.83133700	-0.52069600
C	2.29492500	-0.45919000	-0.77229700
C	1.83808300	1.87714000	-0.07386000
C	1.77153900	3.08631300	-0.31187800
F	1.15137000	0.82360000	2.42168100
F	2.60834900	0.00202900	-1.99632500
H	1.30583400	-1.75006600	2.75930700
H	2.03232500	-3.37372000	0.96690500
H	2.66280300	-2.50817600	-1.31968100
H	1.72396900	4.14103500	-0.52058500
N	-2.32012000	-0.00201000	-0.37359000
C	-1.15073000	-0.57955100	-1.05082200
H	-0.50129500	-1.12452700	-0.32867100
H	-0.54237700	0.24756900	-1.45387600
C	-2.86366100	-0.96094400	0.59646700
H	-2.25216500	-0.97592600	1.53031700
H	-2.78438800	-1.96983700	0.15743300
C	-1.95701600	1.25510400	0.29736300
H	-2.72740600	1.46816800	1.05726400
H	-0.99303400	1.15730500	0.84672800
C	-1.90163500	2.42864500	-0.67787300
H	-1.66467100	3.36327200	-0.14141300
H	-1.12695600	2.28544200	-1.44806500
H	-2.87526800	2.54078100	-1.18201600
C	-1.54863000	-1.49578700	-2.20573500
H	-0.65040900	-1.89026300	-2.71161000
H	-2.14458000	-2.35727500	-1.86141600

H	-2.15282400	-0.93570500	-2.93758200
C	-4.33150600	-0.68884000	0.91931400
H	-4.72238600	-1.44870100	1.61749300
H	-4.47474800	0.29865000	1.38729300
H	-4.92740300	-0.71585400	-0.00709300