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Electronic Supplementary Information for

Electrostatics Control Vibrational Frequencies Shifts in Hydrogen Bonded Complexes!

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Experimental Methodology

Details of experimental setup can be found elsewhere and only a brief outline is presented here.[1] The binary complexes of 3-fluorophenylacetylene (Aldrich) and 2,6-difluorophenylacetylene (Fluorochem, U. K.) with various bases (water, methanol, diethyl ether, ammonia, methylamine, dimethylamine and trimethylamine) were synthesised *in situ* by co-expansion of the required reagents doped in helium buffer gas at 4 atm pressure into a vacuum chamber operating at 10^{-6} Torr. The expansion was carried out using a 0.5 mm diameter pulsed nozzle (Series 9, Iota One; General Valve Corporation) operating at 10 Hz. For recording IR spectra, the species of interest (monomer or the binary complex) were selectively ionized using resonant two-photon ionization method with an UV laser and detected in a two-stage Wiley-McLaren time-of-flight (TOF) mass spectrometer coupled with supersonic jet expansion technique. Prior to the UV laser, an IR laser is introduced, and its wavelength is scanned. When the IR wavelength is resonant with a vibrational transition of the species of interest, the IR absorption induces reduction of the population of the ground state, which is then detected as a decrease in the intensity ion signal intensity.[2] In our experiments the UV laser is a frequency doubled output of a dye laser (Narrow Scan GR; Radiant Dyes) operating with the Rhodamine-19 dye, pumped with second harmonic of a Nd:YAG laser (Surelite I-10; Continuum). The tunable IR laser is an idler component of a $LiNbO_3$ OPO (Custom IR OPO; Euroscan Instruments) pumped with an injection-seeded Nd:YAG laser (Brilliant-B; Quantel). The typical bandwidth of both UV and IR lasers is about 1 cm^{-1} and the absolute frequency calibration is within ±2 cm^{-1}.

Computational Methodology

The C–H···X (X = O, N) hydrogen-bonded complexes of 3FPHA and DFPHA were optimized at MP2/aug-cc-pVDZ level of theory. Geometry optimization was followed vibrational frequency calculations at the same level of theory to evaluate the zero-point energies and the vibrational frequencies of the systems and to verify nature of the minima obtained (presence/absence of imaginary frequencies). The optimized geometries of the

monomers were used for the calculation of stabilization energies. The stabilization energy was determined as the difference between the dimer energy and the sum of monomer energies. The calculated stabilization energies were corrected for the vibrational zero-point energy (ZPE) and the basis-set superposition error (BSSE). The BSSE correction was made after geometry optimization. A scaling factor of 0.958 was chosen so as to match the experimental vibrational frequencies of the monomers and the same scaling factor was used for the complexes. The CCSD(T)/CBS stabilization energies were determined as a sum of MP2/CBS energies and CCSD(T) correction term.

$$\Delta E_{CBS}^{CCSD(T)} = \Delta E_{CBS}^{MP2} + (\Delta E^{CCSD(T)} - \Delta E^{MP2})\Big|_{\text{Medium basis set}} \quad (1)$$

The method takes advantage of the fact that both the CCSD(T) and MP2 methods exhibit approximately the same basis set dependence.[3] Because of different dependence on the basis set the Hartree-Fock energies and MP2 correlation energies were extrapolated separately and using aug-cc-pVDZ (aVDZ) and aug-cc-pVTZ (aVTZ) basis sets. The extrapolations were performed using the method proposed by Helgaker co-workers,[4] wherein the electron-correlation error is proportional to N^{-3} for the aug-cc-pVNZ (aVNZ) basis set.[5]

The analysis of the stabilization energies of various C–H···X hydrogen-bonded complexes was carried out using Symmetry Adapted Perturbation Theory (SAPT).[6] The simplest of SAPT (SAPT0) as well as higher order SAPT (SATP2) approaches were used 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 (density fitting procedures to reduce cost).[7] The perturbative method SAPT0 treats the monomers at the Hartree–Fock level (zero order in the interaction potential) and then dissociates the overall intermolecular interaction energy into the different components using perturbation theory (1st order V in case of electrostatics and exchange, 2nd order V in case of all other interactions). SAPT2 adds electrostatics, exchange, and induction terms up to the second-order with respect to intra-monomer electron correlation while keeping the same SAPT0 treatment for dispersion (orbital relaxations are included). The density fitting approach was used to reduce the computational cost. The main advantage of SAPT calculations is that it allows for the separation of interaction energy 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 equations (2) and (3).

$$E_{SAPT0} = E_{Elec}^{(10)} + E_{Exch}^{(10)} + E_{Ind}^{(20)} + E_{Exch-Ind}^{(20)} + E_{Disp}^{(20)} + E_{Exch-Disp}^{(20)} \quad (2)$$

$$E_{SAPT2} = E_{SAPT0} + E_{Elec}^{(12)} + E_{Exch}^{(11)} + E_{Exch}^{(12)} + {}^{t}E_{Ind}^{(22)} + {}^{t}E_{Exch-Ind}^{(22)} \quad (3)$$

Further, the charge transfer component is given by the equations (4) and (5).[8]

$$E_{Ct}^{(20)} = E_{Ind}^{(20)}(\text{dimer}) - E_{Ind}^{(20)}(\text{monomer}) \quad (4)$$

$$E_{Exch-Ct}^{(20)} = E_{Exch-Ind}^{(20)}(\text{dimer}) - E_{Exch-Ind}^{(20)}(\text{monomer}) \quad (5)$$

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.

Spin component scaled (SCS)-SAPT0 calculations were also carried out and the energy decomposition in this case is given by equation (6).[9]

$$E_{SCS-SAPT0} = E_{SAPT0} - E_{disp}^{(20)} + E_{SCS-disp}^{(20)} \quad (6)$$

Geometry optimization and frequency calculations were carried out using the GAUSSIAN 09 suite of programs,[10] and SAPT calculations were carried out using PSI4 *ab-Initio* package.[11] The structures and the vibrations were visualized by ChemCraft.[12]

Table S1. ZPE and BSSE corrected stabilization energies (kJ mol^{-1}) for various C–H···X hydrogen-bonded complexes of 3FPHA and DFPHA. Scaled vibrational frequencies and their shifts (cm^{-1}) calculated at MP2/aug-cc-pVDZ level of theory.

	ΔE MP2/aVDZ	ΔE MP2/aVTZ	ΔE MP2/CBS	ΔE CCSD(T)/aVDZ	ΔE CCSD(T)/CBS	E_{SAPT2} + ZPE	Calc		Expt	
							ν_{C-H}	$\lvert\Delta\nu_{C-H}\rvert$	ν_{C-H}	$\lvert\Delta\nu_{C-H}\rvert$
3FPHA	--	--	--	--	--	--	3334	--	3336	--
3FPHA-H_2O	-7.0	-8.0	-8.4	-6.9	-8.3	-8.5	3270	64	3287	49
3FPHA-MeOH	-10.5	-11.8	-12.4	-9.9	-11.8	-11.7	3242	92	3267	69
3FPHA-EtOEt	-13.9	-15.8	-16.6	-12.8	-15.5	-14.9	3230	104	3247	89
3FPHA-NH_3	-9.3	-10.6	-11.1	-8.9	-10.7	-11.5	3195	139	3227	109
3FPHA-NH_2Me	-13.0	-14.7	-15.5	-12.0	-14.5	-15.3	3155	179	3192	144
3FPHA-$NHMe_2$	-15.7	-17.9	-18.9	-13.9	-17.1	-18.0	3110	224	3164	172
3FPHA-NMe_3	-14.9	-16.8	-17.6	-13.0	-15.7	-16.9	3065	269	3152	184
DFPHA	--	--	--	--	--	--	3337	--	3335	--
DFPHA-H_2O	-7.6	-8.7	-9.1	-7.3	-8.8	-9.3	3269	68	3277	58
DFPHA-MeOH	-11.1	-12.5	-13.2	-10.3	-12.4	-12.3	3240	97	3260	75
DFPHA-EtOEt	-14.6	-16.6	-17.4	-13.2	-16.0	-15.4	3226	111	3241	94
DFPHA-NH_3	-9.9	-11.3	-11.9	-9.3	-11.3	-12.1	3188	149	3217	118
DFPHA-NH_2Me	-13.7	-15.6	-16.4	-12.4	-15.1	-15.9	3145	192	3180	155
DFPHA-$NHMe_2$	-16.8	-19.1	-20.2	-14.7	-18.1	-18.9	3097	240	3150	185
DFPHA-NMe_3	-16.0	-18.0	-18.9	-13.9	-16.8	-17.8	3050	287	3116	219

Table S2. Stabilization energies (kJ mol^{-1}) for various C–H···X hydrogen-bonded complexes of 3FPHA and DFPHA optimized at MP2/aug-cc-pVDZ level of theory.

	ΔE^a	ΔE^b	ΔE^c	ΔE^d	ΔE^a	ΔE^b	ΔE^c	ΔE^d	E_{SAPT2}	E_{SAPT2} + ZPE
	MP2/aug-cc-pVDZ				MP2/aug-cc-pVTZ					
3FPHA-H_2O	-16.1	-11.6	-11.5	-7.0	-14.5	-10.0	-12.5	-8.0	-13.1	-8.5
3FPHA-MeOH	-19.3	-15.9	-13.9	-10.5	-17.7	-14.4	-15.1	-11.8	-15.0	-11.7
3FPHA-EtOEt	-25.3	-22.2	-17.0	-13.9	-22.8	-19.6	-19.0	-15.8	-18.1	-14.9
3FPHA-NH_3	-21.1	-15.3	-15.1	-9.3	-18.4	-12.6	-16.4	-10.6	-17.3	-11.5
3FPHA-NH_2Me	-24.8	-20.3	-17.5	-13.0	-22.0	-17.4	-19.3	-14.7	-19.9	-15.3
3FPHA-$NHMe_2$	-28.6	-24.5	-19.8	-15.7	-25.7	-21.5	-22.1	-17.9	-22.2	-18.0
3FPHA-NMe_3	-30.4	-25.6	-19.7	-14.9	-25.9	-21.0	-21.7	-16.8	-21.8	-16.9
DFPHA-H_2O	-16.6	-12.2	-12.0	-7.6	-15.0	-10.7	-13.0	-8.7	-13.6	-9.3
DFPHA-MeOH	-20.1	-16.6	-14.6	-11.1	-18.6	-15.1	-16.0	-12.5	-15.8	-12.3
DFPHA-EtOEt	-26.3	-23.1	-17.8	-14.6	-23.9	-20.8	-19.7	-16.6	-18.6	-15.4
DFPHA-NH_3	-22.0	-16.0	-15.9	-9.9	-19.3	-13.4	-17.2	-11.3	-18.0	-12.1
DFPHA-NH_2Me	-26.0	-21.2	-18.5	-13.7	-23.3	-18.5	-20.4	-15.6	-20.7	-15.9
DFPHA-$NHMe_2$	-29.9	-25.8	-20.9	-16.8	-27.2	-23.1	-23.2	-19.1	-23.0	-18.9
DFPHA-NMe_3	-31.8	-27.0	-20.8	-16.0	-27.0	-22.2	-22.8	-18.0	-22.6	-17.8

[a] Electronic stabilization energy
[b] Electronic stabilization energy with ZPE correction
[c] Electronic stabilization energy with BSSE correction
[d] Electronic stabilization energy with ZPE and BSSE corrections

Table S3. SAPT0 interaction energy components (kJ mol^{-1}) for various C–H···X hydrogen-bonded complexes of 3FPHA and DFPHA.

	E_{Elec}	E_{Ind}	E_{Ct}	E_{Disp}	E_{Exch}	E_{SAPT0}	$E_{SCS\text{-}Disp}$	$E_{SCS\text{-}SAPT0}$
3FPHA-H_2O	-20.5	-5.2	-0.9	-5.8	15.5	-15.9	-4.5	-14.7
3FPHA-MeOH	-23.5	-6.6	-1.2	-9.5	21.5	-18.1	-7.4	-16.0
3FPHA-EtOEt	-26.6	-8.3	-1.4	-15.2	27.9	-22.2	-11.9	-18.9
3FPHA-NH_3	-28.7	-8.6	-1.3	-7.7	25.1	-20.0	-6.2	-18.4
3FPHA-NH_2Me	-32.3	-10.8	-1.6	-12.2	32.8	-22.6	-9.7	-20.1
3FPHA-$NHMe_2$	-36.7	-13.5	-2.0	-17.4	42.5	-25.1	-13.7	-21.4
3FPHA-NMe_3	-40.1	-15.5	-1.9	-16.9	47.2	-25.3	-13.4	-21.8
DFPHA-H_2O	-20.7	-5.4	-0.9	-5.9	16.1	-16.0	-4.7	-14.7
DFPHA-MeOH	-24.3	-7.0	-1.3	-10.1	22.8	-18.5	-7.9	-16.3
DFPHA-EtOEt	-27.4	-8.7	-1.5	-15.5	29.2	-22.5	-12.2	-19.1
DFPHA-NH_3	-29.7	-9.1	-1.3	-8.0	26.5	-20.3	-6.4	-18.7
DFPHA-NH_2Me	-33.7	-11.5	-1.8	-12.9	34.8	-23.2	-10.2	-20.5
DFPHA-$NHMe_2$	-38.3	-14.4	-2.1	-17.9	44.8	-25.8	-14.1	-22.0
DFPHA-NMe_3	-41.9	-16.5	-2.0	-17.4	49.8	-27.0	-13.8	-22.4

Note: $E_{SAPT0} = E_{Elec} + E_{Ind} + E_{Disp} + E_{Exch}$. E_{Ct} is given by the eqn.s (4) and (5).

Table S4. SAPT2 interaction energy components (kJ mol^{-1}) for various C–H···X hydrogen-bonded complexes of 3FPHA and DFPHA.

	E_{Elec}	E_{Ind}	E_{Ct}	E_{Disp}	E_{Exch}	E_{SAPT2}
3FPHA-H_2O	-18.8	-5.3	-1.1	-5.8	16.7	-13.1
3FPHA-MeOH	-22.7	-7.0	-1.6	-9.5	24.1	-15. 0
3FPHA-EtOEt	-25.5	-8.7	-1.8	-15.2	31.3	-18.1
3FPHA-NH_3	-27.7	-8.9	-1.6	-7.7	27.0	-17.3
3FPHA-NH_2Me	-32.1	-11.2	-2.1	-12.2	35.7	-19.9
3FPHA-$NHMe_2$	-37.1	-14.1	-2.5	-17.4	46.4	-22.2
3FPHA-NMe_3	-40.6	-16.2	-2.5	-16.9	52.0	-21.8
DFPHA-H_2O	-19.9	-5.6	-1.2	-5.9	17.7	-13.6
DFPHA-MeOH	-23.8	-7.3	-1.7	-10.1	25.5	-15.8
DFPHA-EtOEt	-26.6	-9.2	-1.9	-15.5	32.8	-18.6
DFPHA-NH_3	-29.1	-9.4	-1.7	-8.0	28.5	-18.0
DFPHA-NH_2Me	-33.0	-11.9	-2.2	-12.9	37.9	-20.7
DFPHA-$NHMe_2$	-39.0	-15.0	-2.6	-17.9	48.9	-23.0
DFPHA-NMe_3	-42.8	-17.2	-2.7	-17.4	54.8	-22.6

Note: $E_{SAPT0} = E_{Elec} + E_{Ind} + E_{Disp} + E_{Exch}$. E_{Ct} is given by the eqn.s (4) and (5).

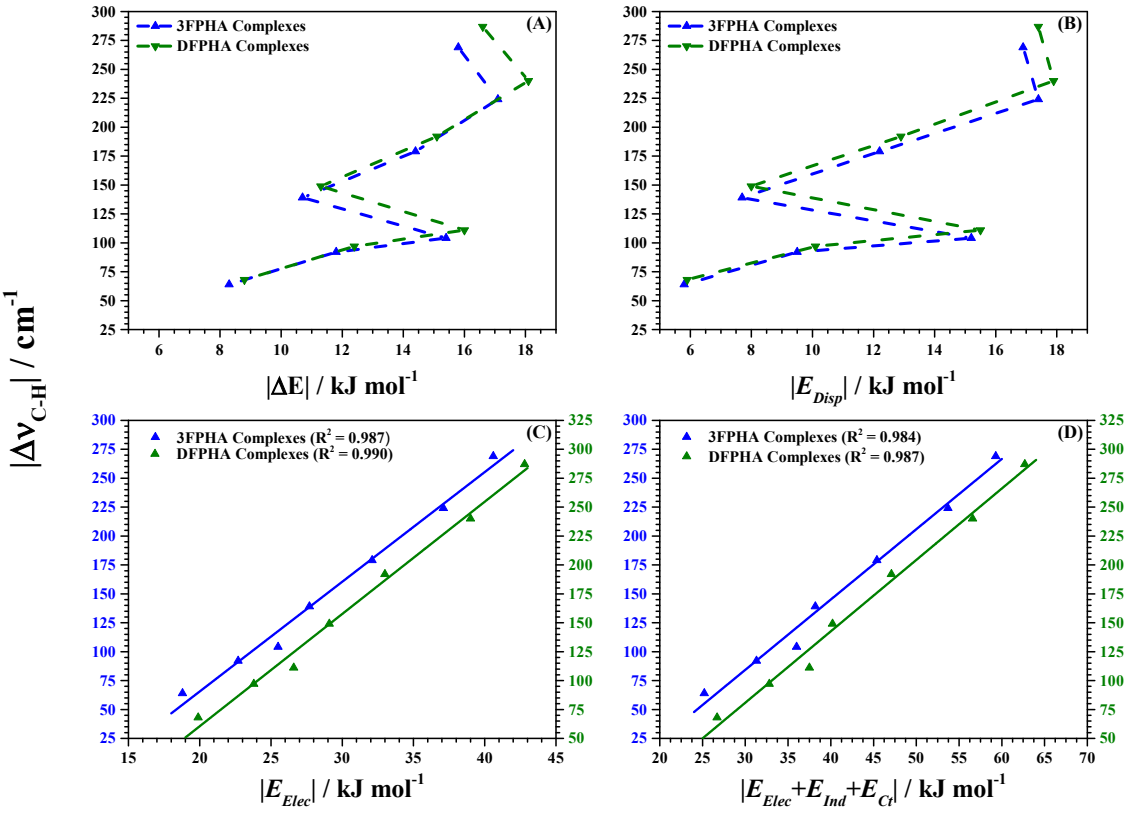

Fig. 1S. Plot of red-shift in the acetylenic C–H stretching frequency in several hydrogen-bonded complexes of 3FPHA and DFPHA with (A) CCSD(T)/CBS stabilization energy, (B) dispersion energy, (C) electrostatic energy and (D) sum of electrostatic, induction and charge-transfer energies. In (A) and (B) dashed are trend lines, while in (C) and (D) the solid lines are linear fits to the data points. In (C) and (D) the y-scales for the 3FPHA (▲) and DFPHA (▲)are shifted relative to each other for clarity.

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Optimized coordinates of 3-fluorophenylacetylene (3FPHA) and 2,6-difluorophenylacetylene (DFPHA) with several Lewis bases

3FPHA-H_2O

C	0.05490100	0.27735600	-0.00001000
C	0.87660200	-0.87550700	0.00000000
C	2.26222000	-0.70401500	0.00000800
C	2.87666900	0.55301100	0.00000900
C	2.04815400	1.69132700	-0.00000600
C	0.64952800	1.56264200	-0.00001800
C	-1.37696400	0.13682800	-0.00002700
C	-2.60892400	0.01964100	-0.00004400
H	3.96647400	0.62826500	0.00001900
H	2.50228800	2.68631100	-0.00000900
H	-3.68349100	-0.08469300	-0.00004200
H	0.00782700	2.44729900	-0.00003300
H	0.44303700	-1.87810900	0.00000200
F	3.05506300	-1.81889200	0.00002800
O	-5.83317900	-0.29366700	-0.00003000
H	-6.37984300	-0.52439700	-0.76203900
H	-6.37954600	-0.52300600	0.76261200

3FPHA-MeOH

C	0.65204800	0.33818300	-0.15768800
C	1.42277000	-0.84939200	-0.16070200
C	2.80160600	-0.74724400	0.03346500
C	3.45719200	0.47303200	0.23048000
C	2.67921700	1.64646900	0.23098000
C	1.28906800	1.58758500	0.03934600

C	-0.77143500	0.26922600	-0.35408100
C	-1.99698600	0.21471800	-0.51971100
H	4.53946800	0.49408800	0.37735200
H	3.16634400	2.61393600	0.38238100
H	-3.06745200	0.16391400	-0.66238400
H	0.68667200	2.49946000	0.03940000
H	0.95597200	-1.82541100	-0.31127500
F	3.54509600	-1.89551900	0.03044700
O	-5.15556300	0.03436400	-0.48371400
H	-5.82277500	-0.36798100	-1.05451400
C	-5.35788600	-0.45046100	0.85646700
H	-5.25980300	-1.54670000	0.91213000
H	-4.57232900	0.00821700	1.47061500
H	-6.34101900	-0.14744100	1.25064900

3FPHA-Et_2O

C	4.75348600	-0.00357000	0.50093600
C	3.96087700	-0.01186500	1.66452200
C	2.55894200	-0.01133100	1.57938300
C	1.92425500	-0.00236600	0.31322600
C	2.71000300	0.00603000	-0.86460700
C	4.10024700	0.00518200	-0.73635500
C	0.48908100	-0.00171900	0.21734800
C	-0.74650800	-0.00100600	0.13877100
F	4.85812400	0.01332100	-1.87528100
H	5.84512100	-0.00380600	0.54221800
H	4.44581800	-0.01879800	2.64482500
H	1.94507100	-0.01777400	2.48357300

H	2.24542100	0.01303400	-1.85320800
H	-1.82561100	-0.00048200	0.06815200
C	-4.68494200	1.18824600	-0.12979900
O	-3.88682100	0.00058000	-0.06848400
C	-3.75573400	2.38858800	-0.04727100
C	-4.68542500	-1.18609000	-0.14167900
C	-3.75669900	-2.38757100	-0.07116400
H	-5.40880300	1.18701800	0.70841900
H	-5.26027000	1.19486600	-1.07610200
H	-3.18998500	2.37372400	0.89616500
H	-3.04301200	2.38274900	-0.88533200
H	-4.34074900	3.32038700	-0.09086600
H	-5.26075000	-1.18300600	-1.08800300
H	-5.40928900	-1.19295700	0.69650800
H	-4.34208900	-3.31865400	-0.12403200
H	-3.19092300	-2.38234100	0.87235800
H	-3.04399400	-2.37365600	-0.90914400

3FPHA-NH_3

C	-0.06694400	0.27563000	0.00015300
C	-0.66040300	1.56160200	0.00004700
C	-2.05885400	1.69242000	-0.00012400
C	-2.88910300	0.55532700	-0.00008800
C	-2.27619500	-0.70242100	0.00008500
C	-0.89083500	-0.87581100	0.00016300
C	1.36467600	0.13292800	0.00021300
C	2.59716700	0.01352000	0.00006500
F	-3.07069800	-1.81644700	-0.00015500

H	-0.01761000	2.44548900	0.00002300
H	-2.51147300	2.68811400	-0.00026200
H	-3.97880500	0.63206300	-0.00024000
H	-0.45887000	-1.87910800	0.00019800
H	3.67636100	-0.09299200	-0.00004200
N	5.90365500	-0.32392900	-0.00024400
H	6.34953600	0.14211800	-0.79074600
H	6.33939400	0.06122100	0.83803100
H	6.19511300	-1.30054900	-0.04694300

3FPHA-NH_2Me

C	0.64924500	0.33158700	-0.15276200
C	1.28168700	1.58640500	0.02492500
C	2.67300600	1.65523900	0.20432000
C	3.45765300	0.48622900	0.21055700
C	2.80701100	-0.73960500	0.03278000
C	1.42723800	-0.85141900	-0.14875200
C	-0.77531600	0.25228500	-0.33644100
C	-2.00257700	0.18714000	-0.49099300
F	3.55695300	-1.88399500	0.03645300
H	0.67435700	2.49501000	0.01986600
H	3.15591200	2.62706600	0.34076500
H	4.54097100	0.51485500	0.34817900
H	0.96472200	-1.83167000	-0.28436300
H	-3.07904600	0.12794300	-0.62678900
N	-5.22365200	-0.07473600	-0.53101500
C	-5.26968400	-0.39742200	0.90837600

H	-5.78675800	0.75417600	-0.72084900
H	-5.64711500	-0.82907500	-1.07130100
H	-4.66252600	-1.29627800	1.09060900
H	-6.28335100	-0.57487600	1.30818000
H	-4.81374500	0.42931200	1.47267100

3FPHA-NHMe$_2$

C	-1.12024700	-0.41463800	-0.17441600
C	-1.79593900	0.81940100	-0.01504300
C	-3.18442600	0.80373800	0.12995000
C	-3.93999700	-0.37384300	0.12505700
C	-3.25645700	-1.59438100	-0.03431800
C	-1.86011500	-1.62241100	-0.18308300
C	0.31002900	-0.43482300	-0.32549700
C	1.54162900	-0.45857000	-0.45898100
H	-5.02507700	-0.32720000	0.24234400
H	-3.82263500	-2.53013300	-0.04215600
H	2.62565800	-0.46936200	-0.56286500
H	-1.33119900	-2.57072600	-0.30701600
H	-1.24951500	1.76519900	-0.00565100
F	-3.83535300	1.99728700	0.28387800
N	4.66095000	-0.14673600	-0.32126000
H	5.43367100	-0.52562500	-0.86772300
C	4.78977600	-0.58783700	1.07224700
H	3.88798000	-0.27922200	1.62587700
H	4.85378800	-1.68524800	1.10969000
H	5.67218000	-0.15972100	1.58900800
C	4.66616000	1.31693900	-0.42399400

H	4.63840100	1.61481200	-1.48243800
H	3.75959400	1.70905600	0.06531400
H	5.54619900	1.78828000	0.05800500

3FPHA-NMe$_3$

C	-1.62057100	-0.31614200	-0.00113000
C	-2.40956200	0.85964500	-0.00084400
C	-3.79952800	0.72839600	0.00034000
C	-4.45011000	-0.51033300	0.00120800
C	-3.65469800	-1.67210400	0.00092000
C	-2.25294000	-1.58361000	-0.00025500
C	-0.18560500	-0.21682200	-0.00242800
C	1.05092200	-0.13508400	-0.00367500
H	-5.54164600	-0.55409900	0.00211900
H	-4.13730200	-2.65359900	0.00159200
H	2.14020900	-0.06033500	-0.00441900
H	-1.63711700	-2.48651000	-0.00045200
H	-1.94743200	1.84942000	-0.00145100
F	-4.55995400	1.86583200	0.00063500
N	4.19073200	0.09158700	0.00037300
C	4.67370000	-0.11794000	1.36578300
H	4.22986200	0.63656000	2.03341500
H	4.36932400	-1.11661200	1.71512100
H	5.78145800	-0.04237600	1.43473400
C	4.55457300	1.42966200	-0.46747800
H	4.16047400	1.58452300	-1.48373600
H	4.11172900	2.18600300	0.19876900
H	5.65652900	1.58058600	-0.48942600

C	4.74089700	-0.92660000	-0.89523100
H	4.43739300	-1.92608400	-0.54742100
H	4.34656000	-0.77499600	-1.91187400
H	5.85195100	-0.89049100	-0.93856700

DFPHA-H_2O

C	1.07596300	1.19549800	-0.00025600
C	2.47209900	1.22243700	0.00522600
C	3.16844100	0.00024800	0.00787500
C	2.47237000	-1.22209500	0.00513700
C	1.07622700	-1.19546500	-0.00033600
C	0.32576800	-0.00006500	-0.00335300
F	0.39588300	2.37337400	-0.00274800
F	0.39641000	-2.37348900	-0.00292200
C	-1.10514800	-0.00022200	-0.00936600
C	-2.34128800	-0.00032600	-0.01448100
H	2.99069000	2.18344200	0.00725700
H	4.26141000	0.00036900	0.01210400
H	2.99117400	-2.18298600	0.00709700
H	-3.42105800	-0.00039600	-0.01799200
O	-5.56667200	-0.00011300	-0.01752900
H	-6.14328600	-0.76185000	0.12369800
H	-6.14279200	0.76331100	0.11642200

DFPHA-MeOH

C	-0.82710000	-0.12095100	-0.01140100
C	-1.80721300	-1.13637200	0.01272600
C	-3.17874100	-0.87443200	0.03063700

C	-3.60806000	0.46508900	0.02458700
C	-2.67522500	1.51775300	0.00106600
C	-1.31489800	1.20340300	-0.01607800
C	0.57301600	-0.41464200	-0.03048100
C	1.78420400	-0.66268900	-0.04972500
H	-4.67748800	0.69029700	0.03817100
H	-2.98497600	2.56487500	-0.00406600
H	2.84601500	-0.86633600	-0.06348400
O	4.92110100	-0.66138400	-0.13136100
H	5.64641000	-1.14353400	0.28602400
C	5.11510500	0.74454200	0.11194900
H	6.04362000	1.10918200	-0.35555200
H	4.26024000	1.25688900	-0.34792100
H	5.12963800	0.97255400	1.18993000
F	-0.40614500	2.21582900	-0.03867300
F	-1.38434700	-2.42865400	0.01860800
H	-3.88435900	-1.70763600	0.04870200

DFPHA-Et_2O

C	1.97482400	-0.00004500	0.00005800
C	2.72531000	-1.05874900	-0.55536400
C	4.12142600	-1.08240600	-0.56786700
C	4.81771800	-0.00002200	-0.00007600
C	4.12146400	1.08235200	0.56778300
C	2.72534600	1.05867200	0.55541300
C	0.54430500	-0.00005600	0.00012900
C	-0.69242300	-0.00005500	0.00019800
H	5.91069300	-0.00001400	-0.00012800

H	4.64022800	1.93330400	1.01411800
H	-1.77417700	-0.00004300	0.00022800
O	-3.82408900	0.00024300	0.00010200
C	-4.62469800	0.66662500	-0.98302800
H	-5.27711400	1.40847900	-0.48255000
C	-4.62501200	-0.66708600	0.98233200
H	-5.27603100	-1.40967500	0.48112400
H	-5.27728900	0.07216900	1.48682300
C	-3.69232100	-1.34072100	1.97604800
H	-4.27916000	-1.86409700	2.74681400
H	-3.05058400	-2.07450100	1.46599200
H	-3.05164000	-0.59497100	2.46981500
C	-3.69168600	1.34130200	-1.97573700
H	-4.27827700	1.86408600	-2.74709400
H	-3.05127500	2.07574000	-1.46496500
H	-3.04968600	0.59626900	-2.46887400
H	-5.27557500	-0.07338500	-1.48822000
H	4.64016000	-1.93335000	-1.01425000
F	2.04534800	-2.10190500	-1.10249900
F	2.04542100	2.10181500	1.10261300

DFPHA-NH_3

C	-0.33576800	-0.00038100	0.00014100
C	-1.08605500	1.19526900	-0.00000600
C	-2.48223500	1.22300800	-0.00025900
C	-3.17948200	0.00132500	-0.00038600
C	-2.48369600	-1.22118900	-0.00026000
C	-1.08748400	-1.19513300	-0.00000600

C	1.09507000	-0.00120400	0.00046800
C	2.33195800	-0.00149200	0.00120100
H	-4.27246200	0.00197200	-0.00058600
H	-3.00266200	-2.18202100	-0.00035700
H	3.41688000	-0.00201700	0.00117000
N	5.63772500	0.00020200	-0.00081300
H	6.03032700	-0.21773400	0.91533100
H	6.03058200	0.90263300	-0.26958900
H	6.03153600	-0.68380800	-0.64734000
H	-3.00004700	2.18446100	-0.00035500
F	-0.40876100	-2.37400300	0.00011500
F	-0.40591400	2.37332400	0.00011500

DFPHA-NH_2Me

C	-1.35080900	1.20270400	-0.00000800
C	-2.71867600	1.48332400	-0.00005700
C	-3.62569900	0.40809300	-0.00005600
C	-3.16311100	-0.92032400	-0.00001700
C	-1.78533900	-1.14805600	0.00002000
C	-0.82968400	-0.10909400	0.00002900
F	-0.46784800	2.23798100	-0.00000300
F	-1.33147400	-2.43007800	0.00008200
C	0.57726400	-0.36835300	0.00006700
C	1.79493400	-0.58785600	0.00000400
H	-3.05391400	2.52260400	-0.00008700
H	-4.70046300	0.60677500	-0.00008700
H	-3.84783900	-1.77098700	-0.00001400
H	2.86659100	-0.77118700	-0.00000900

C	5.06410900	0.78998000	0.00018500
N	5.00170000	-0.68481600	-0.00023200
H	4.53442300	1.16830600	-0.88640600
H	6.08631700	1.20678200	0.00022000
H	4.53456900	1.16780000	0.88707800
H	5.49226300	-1.05526200	0.81360800
H	5.49210800	-1.05475500	-0.81439500

DFPHA-NHMe$_2$

C	1.23733500	-0.08719800	-0.08398000
C	1.78939600	1.20363800	0.06232800
C	3.15907700	1.44003700	0.19552600
C	4.03549600	0.33973300	0.18417100
C	3.54128100	-0.96955400	0.04181600
C	2.16300100	-1.15296100	-0.08776400
C	-0.17074600	-0.30051600	-0.21847300
C	-1.38878200	-0.48404500	-0.33940300
H	5.11120300	0.50377000	0.28683900
H	4.20206200	-1.83886800	0.03011400
H	-2.46529800	-0.62730700	-0.43110300
N	-4.50630300	-0.42913700	-0.25809900
H	-5.23657600	-0.99466300	-0.68949100
H	3.51933500	2.46507700	0.30485500
F	1.67836100	-2.41615900	-0.22545000
F	0.93558400	2.26309800	0.07280800
C	-4.63155600	0.95905700	-0.71736000
H	-3.76689000	1.53378200	-0.34708900
H	-4.61521800	0.98892400	-1.81673600

H	-5.55393400	1.45853200	-0.35881400
C	-4.61704900	-0.52414700	1.20204000
H	-4.58838900	-1.58011300	1.50846400
H	-3.75268500	-0.01273600	1.65634200
H	-5.53970400	-0.05915200	1.60369100

DFPHA-NMe_3

C	-1.69968700	0.00042200	-0.00305900
C	-2.45140800	1.19526600	-0.00101200
C	-3.84758900	1.22140900	0.00255800
C	-4.54344400	-0.00112800	0.00438600
C	-3.84625400	-1.22290700	0.00256900
C	-2.45009900	-1.19525700	-0.00100400
C	-0.26918000	0.00115300	-0.00690100
C	0.96871900	0.00112900	-0.01100100
H	-5.63642900	-0.00173500	0.00718300
H	-4.36424500	-2.18423700	0.00394500
H	2.06150000	0.00128100	-0.01347400
N	4.09955000	0.00022400	-0.00103800
H	-4.36663400	2.18217300	0.00393700
F	-1.76995600	-2.37336000	-0.00271800
F	-1.77252700	2.37409300	-0.00268900
C	4.57242900	1.31799100	-0.42753200
H	4.20230200	1.53177300	-1.44210100
H	4.18334000	2.08798900	0.25634000
H	5.68298400	1.38161400	-0.43601100
C	4.57618300	-1.03354300	-0.92083600
H	4.19018500	-2.01468200	-0.60407100

H	4.20574400	-0.82271600	-1.93590600
H	5.68692900	-1.08476200	-0.95379200
C	4.54981400	-0.28504700	1.36195700
H	4.16026400	0.48367400	2.04705900
H	4.16340600	-1.26564500	1.68003300
H	5.65924100	-0.29981100	1.44202700
