Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Solvation stabilizes intercarbonyl n→π* interactions and polyproline II helix

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Table S1. Comparison of calculated formaldehyde dimer interaction energies (ΔE_{int}) using either the MP2 method or the CCSD(T) method, with the jul-cc-pV5Z basis set in implicit water. These energies do not include a correction for basis-set superposition error (BSSE).

	groups on C=O			ΔE_{int}, kcal mol^{-1} jul-cc-pV5Z implicit H_2O	
interaction	**donor**	**acceptor**	***d***	**MP2**	**CCSD(T)**
HCHO·HCHO	**–**	**–**	2.835	-1.40	-1.38
HCHO·HCHO	**HF**	**–**	2.883	-1.20	-1.18
HCHO·HCHO	**–**	**HF**	2.677	-2.05	-2.03
HCHO·HCHO	**–**	**H^+**	1.567	-18.01	-17.45
HCHO·HCHO	**–**	**Li^+**	2.714	-2.20	-1.96
HCHO·HCHO	**–**	**Na^+**	2.760	-1.80	-1.78
HCHO·HCHO	**–**	**K^+**	2.781	-1.63	-1.61

Table S2. Energies of small molecules and of the formaldehyde dimer as a function of explicit solvation. Structures were generated via geometry optimization using the MP2 method with the aug-cc-pVTZ basis set in implicit water (IEFPCM). Energies and dipole moments (μ, Debye (D)) were determined using the MP2 method with the jul-cc-pV5Z basis set in implicit water.

structure	solvation: donor C=O	solvation: acceptor C=O	μ, D	*E*, hartrees	hydrogen bond energy (H_2O), kcal mol^{-1}	n–>π^* interaction energy (H_2O), ΔE_{int}, kcal mol^{-1}
small molecules						
HF			2.1	-100.3858432		
H_2O			2.3	-76.3666412		
HCHO			3.6	-114.3652428		
urea			6.0	-225.0111957		
thiourea			8.1	-547.5833603		
guanidinium			0.1	-205.5741383		
H_2O•H_2O (lower dipole moment structure)			3.6	-152.7396691	-4.01 [a]	
H_2O•H_2O (higher dipole moment structure)			4.9	-152.7396744	-4.01 [a]	
solvated formaldehyde						
HCHO	HF		6.2	-214.7636148	-7.86	
HCHO	HF HF		7.4	-315.1584774	-13.52	
HCHO	HF HF HF		8.4	-415.5438695	-13.24	
HCHO	HF HF HF HF		9.6	-515.9300256	-13.43	
HCHO	H_2O		5.2	-190.7376407	-3.61	
HCHO	H_2O H_2O		6.8	-267.1093588	-6.80	
HCHO	urea		10.4	-339.3835702	-4.48	
HCHO	thiourea		12.8	-661.9568991	-5.21	
HCHO	guanidinium		1.7	-319.9495627	-6.39	
HCHO	H^+		2.7	-114.7493453		
HCHO	Li^+		7.5	-121.7978689		
HCHO	Na^+		5.7	-276.2029433		
HCHO	K^+		6.1	-713.5084525	[b]	
formaldehyde dimer						
HCHO•HCHO	–	–	7.3	-228.7327149		-1.40
HCHO•HCHO	HF	–	9.7	-329.1307738		-1.20 [c]
HCHO•HCHO	–	HF	9.8	-329.1321248		-2.05
HCHO•HCHO	HF	HF	12.4	-429.5298231		-1.63
HCHO•HCHO	–	HF HF	11.2	-429.5281456		-2.78
HCHO•HCHO	HF	HF HF	13.7	-529.9254490		-2.11
HCHO•HCHO	H_2O	–	8.6	-305.1050026		-1.33
HCHO•HCHO	–	H_2O	8.5	-305.1055694		-1.69
HCHO•HCHO	–	H_2O H_2O	9.2	-381.4777857		-2.00
HCHO•HCHO	H_2O	H_2O	10.2	-381.4779789		-1.69
HCHO•HCHO	HF	H_2O H_2O	11.2	-481.8756297		-1.67
HCHO•HCHO	H_2O	H_2O H_2O	10.6	-457.8502724		-2.05
HCHO•HCHO	–	urea	14.2	-453.7516156		-1.76
HCHO•HCHO	–	thiourea	16.7	-776.3250734		-1.84
HCHO•HCHO	–	guanidinium	4.1	-434.3180239		-2.02
HCHO•HCHO	–	H^+	4.6	-229.1432872		-18.01
HCHO•HCHO	–	Li^+	9.8	-236.1666230		-2.20
HCHO•HCHO	–	Na^+	9.0	-390.5710589		-1.80
HCHO•HCHO	–	K^+	8.0	-827.8762935	[b]	-1.63

[a] Two structures of the hydrogen-bonded water dimer were analyzed: one with a lower overall dipole moment (non-hydrogen-bonded hydrogen atoms pointed in opposite directions, which is the energy minimum in the gas phase; 3.5 Debye in water) and one with a higher overall dipole moment (non-hydrogen-bonded hydrogen atoms pointed in the same direction; 4.8 Debye in

water). While these structures differ significantly in energy in the gas phase (counterpoise BSSE-corrected interaction energies of –4.85 and –4.22 kcal mol^{-1}, respectively), the interaction energies are identical in implicit water (–4.01 and –4.01 kcal mol^{-1}, respectively). These energies were determined by the MP2 method with the jul-cc-pV5Z basis set, on the structures optimized by the MP2 method with the aug-cc-pVTZ basis set in implicit water. Using the CCSD(T) method and the jul-cc-pV5Z basis set in implicit water, similar interaction energies were also obtained (–4.01 and –4.00 kcal mol^{-1}, respectively).

For the water dimer structures, hydrogen bond energies were determined by subtracting the energy of two water molecules from the energy of the water dimer:

$$\Delta E_{\text{H-bond}} = E_{\text{H2O dimer}} - 2E_{\text{H2O}}$$

For solvated formaldehyde, hydrogen bond energies were determined by subtracting the energy of formaldehyde and the energy (energies) of the individual solvating hydrogen-bond donor molecule(s) from the energy of the hydrogen-bonded complex:

$$\Delta E_{\text{H-bond}} = E_{\text{complex}} - E_{\text{HCHO}} - \Sigma\, E_{\text{solvating molecules}}$$

[b] For structures with K^+, the 6-311++G(3d,3p) basis set was used for K and the aug-cc-pVTZ basis set was used for all other atoms in geometry optimization; and the Def2QZVP basis set was used for K and the jul-cc-pV5Z basis set was used for all other atoms in energy calculations.

[c] n→π* interaction energies were determined by subtracting the energies of the component solvated formaldehyde molecules from the total energy of the formaldehyde dimer complex:

$$\Delta E_{\text{interaction}} = \Delta E_{\text{int}} = E_{\text{complex}} - E_{\text{solvated HCHO donor C=O}} - E_{\text{solvated HCHO acceptor C=O}}$$

Thus, for example, for the complex [HCHO•••HCHO(HF)], the n→π* interaction energy is $\Delta E_{\text{int}} = E_{\text{complex}} - E_{\text{HCHO}} - E_{\text{HCHO(HF)}}$; and for the complex [HCHO(HF)•••HCHO(HFHF)], the n→π* interaction energy is $\Delta E_{\text{int}} = E_{\text{complex}} - E_{\text{HCHO(HF)}} - E_{\text{HCHO(HFHF)}}$.

Table S3. Comparison of different methods to calculate pyramidalization of the electron-acceptor carbonyl.[a]

interaction			groups on C=O: donor	groups on C=O: acceptor	pyramidalization, acceptor C=O: Δ, °	$d\Delta$, Å	θ, °	$d'\Delta$, Å	$d_{C=O}$, Å
HCHO·HCHO			–	–	0.6	0.006	0.9	0.019	1.217
HCHO·HCHO			H_2O	–	0.5	0.004	0.6	0.013	1.217
HCHO·HCHO			–	H_2O	0.7	0.008	1.1	0.024	1.220
HCHO·HCHO			–	H_2O H_2O	1.0	0.009	1.4	0.029	1.223
HCHO·HCHO			H_2O	H_2O	0.3	0.003	0.5	0.010	1.221
HCHO·HCHO			H_2O	H_2O H_2O	0.4	0.005	0.7	0.014	1.222
HCHO·HCHO			HF	–	0.4	0.004	0.6	0.012	1.217
HCHO·HCHO			–	HF	1.1	0.010	1.5	0.033	1.224
HCHO·HCHO			–	HF HF	1.6	0.016	2.4	0.052	1.228
HCHO·HCHO			HF	HF	0.5	0.005	0.7	0.015	1.222
HCHO·HCHO			HF	HF HF	0.7	0.008	1.1	0.024	1.228
HCHO·HCHO			–	urea	0.8	0.009	1.3	0.028	1.220
HCHO·HCHO			–	thiourea	0.9	0.009	1.3	0.028	1.220
HCHO·HCHO			–	guanidinium	0.9	0.009	1.4	0.029	1.222
HCHO·HCHO			–	Li^+	0.9	0.009	1.3	0.028	1.221
HCHO·HCHO			–	Na^+	0.7	0.007	1.1	0.023	1.222
HCHO·HCHO			–	K^+	0.6	0.005	0.8	0.017	1.218
Ac-Pro-NMe_2	*exo*	PPII	–	–	2.1	0.022	2.7	0.058	1.227
Ac-Pro-NMe_2	*endo*	PPII	–	–	1.4	0.015	1.9	0.040	1.227
Ac-Pro-NMe_2	*exo*	α	–	–	–1.7	0.019	2.4	0.052	1.230
Ac-Pro-NMe_2	*endo*	α	–	–	–0.5	0.006	0.7	0.016	1.232
Ac-Ala-NMe_2		PPII	–	–	2.0	0.021	2.6	0.056	1.227
Ac-Ala-NMe_2		PPII	–	HF HF	2.4	0.027	3.4	0.074	1.261
Ac-Ala-NMe_2		α	–	–	–0.7	0.008	1.0	0.021	1.229
Ac-Ala-NMe_2		α	–	HF HF	–0.8	0.009	1.1	0.025	1.263

[a] Δ = pyramidalization of the carbonyl, as defined by the torsion angle (°) between the *pro-R* H, the *pro-S* H, the carbonyl O, and the carbonyl C for formaldehyde complexes (shown schematically in Figure 1c), and as defined by the torsion angle between the Cα, the N of the dimethyl amide, the carbonyl O, and the carbonyl C for peptides. Three other methods to quantify pyramidalization were also examined: (1) $d\Delta$, the orthogonal distance between the C of the carbonyl and the plane defined by other three atoms attached to the carbonyl C; (2) θ, the angle between the bond of the carbonyl and the plane defined by the carbonyl C and the non-O atoms attached to the carbonyl; and (3) $d'\Delta$, the orthogonal distance between the O of the carbonyl and the plane defined by the carbonyl C and the non-O atoms attached to the carbonyl. The torsion angle-based determination of the extent of pyramidalization (Δ) was used as the primary method, as it can be rapidly conducted in popular molecular graphics programs (e.g. GaussView or Pymol). The other methods involved defining the atoms of the plane (here, conducted in Mercury) and then calculating the distance of those atoms to the plane. $\theta = \sin^{-1}(d'\Delta / d_{C=O})$, where $d_{C=O}$ = the length of the C=O bond (Å). In contrast to other approaches, the torsion angle-based measurement (Δ) has the specific advantage of indicating the stereochemistry of the puckering of the carbonyl C: for the formaldehyde complexes, and for peptides in a PPII conformation, with the torsion angles as defined, an n→π* interaction would be expected to have a positive value of Δ, while for peptides in an α conformation, a negative value of Δ is expected. In all cases herein, the sign of Δ matched the expectations for the relevant n→π* interaction.

Table S4. Energies of Ac-Pro-NMe_2 as a function of ring pucker, main chain conformation, and explicit solvation. Structures of all molecules were generated via geometry optimization using the M06-2X method with the jun-cc-pVTZ basis set in implicit water (IEFPCM). Energies and dipole moments (μ, Debye (D)) were determined using the MP2 method with the aug-cc-pVTZ basis set in implicit water.

			solvation			*E*	E_{rel} [a]
	pucker	*2°*	donor	acceptor	μ, D	hartrees	kcal mol^{-1}
Ac-Pro-NMe_2	*exo*	*PPII*	–	–	6.8	-611.4427653	0.48
			–	HF *cis*	9.2	-711.8111236	0.34
			–	HF *trans*	10.0	-711.8082455	0.37
			–	HF HF	11.6	-812.1726305	0.15
			HF	–	10.9	-711.8103764	0.55
			HF	HF HF	14.3	-912.5390250	0.24
			–	urea	12.8	-836.3853222	-0.66
			–	thiourea	14.6	-1158.9660345	-1.35
			–	guanidinium	9.1	-816.9609505	-1.13
			–	H_2O *cis*	7.1	-687.7906696	0.57
			–	H_2O HF	9.7	-788.1543161	0.47
			HFHF	HF HF	14.5	-1012.8995328	0.68
			HFHF	–	12.0	-812.1722480	0.92
			–	5 H2O	11.5	-993.1819748	-0.34
	endo	*PPII*	–	–	6.8	-611.4435351	*0.00*
			–	HF *cis*	9.3	-711.8116707	*0.00*
			–	HF *trans*	9.8	-711.8088360	*0.00*
			–	HF HF	11.6	-812.1728646	*0.00*
			HF	–	11.2	-711.8112481	*0.00*
			HF	HF HF	14.4	-912.5394072	*0.00*
			–	urea	12.8	-836.3842636	*0.00*
			–	thiourea	12.4	-1158.9638841	*0.00*
			–	guanidinium	11.7	-816.9591571	*0.00*
			–	H_2O *cis*	7.3	-687.7915841	*0.00*
			–	H_2O HF	9.9	-788.1550576	*0.00*
			HFHF	HF HF	15.9	-1012.9006178	*0.00*
			HFHF	–	12.2	-812.1737124	*0.00*
			–	5 H2O	14.3	-993.1812713	*0.00*
	exo	*α*	–	–	10.4	-611.4409817	1.60
			–	HF *cis*	13.2	-711.8086470	1.90
			–	HF *trans*	14.0	-711.8068750	1.23
			–	HF HF	15.8	-812.1700338	1.78
			HF	–	13.1	-711.8082548	1.88
			HF	HF HF	17.7	-912.5358943	2.20
			–	urea	17.4	-836.3787901	3.43
			–	thiourea	19.9	-1158.9584948	3.38
			–	guanidinium	9.6	-816.9550503	2.58
			–	H_2O *cis*	10.9	-687.7872968	2.69
			–	H_2O HF	13.1	-788.1509384	2.58
			HFHF	HF HF	19.7	-1012.8946023	3.77
			HFHF	–	15.4	-812.1680689	3.54
	endo	*α*	–	–	9.8	-611.4381338	3.39
			–	HF *cis*	12.7	-711.8056418	3.78
			–	HF *trans*	13.0	-711.8037168	3.21
			–	HF HF	14.8	-812.1668643	3.77
			HF	–	12.3	-711.8050265	3.90
			HF	HF HF	15.7	-912.5327228	4.19
			–	urea	16.5	-836.3758769	5.26
			–	thiourea	18.8	-1158.9555368	5.24
			–	guanidinium	12.7	-816.9519974	4.49
			–	H_2O *cis*	9.3	-687.7843326	4.55
			–	H_2O HF	12.1	-788.1479774	4.44
			HFHF	HF HF	17.7	-1012.8926256	5.02
			HFHF	–	14.2	-812.1653645	5.24

[a] Relative energies (E_{rel}) are referenced to the energy of the structure with an *endo* ring pucker and PPII conformation with the given solvation pattern (italics). All structures have *trans* Ac-Pro amide bonds.

Table S5. Energies of Ac-Ala-NMe_2 as a function of main chain conformation and explicit solvation. Structures of all molecules were generated via geometry optimization using the M06-2X method with the jun-cc-pVTZ basis set in implicit water (IEFPCM). Energies and dipole moments (μ, Debye (D)) were determined using the MP2 method with the aug-cc-pVTZ basis set in implicit water.

		C=O solvation			*E*,	E_{rel} [a], kcal mol^{-1}		
	2°	donor	acceptor	μ, D	hartrees	to α	to PPII	to β
Ac-Ala-NMe2	**PPII**	–	–	5.1	-534.1925525	-1.69	*0.00*	0.91
		–	HF HF	9.5	-734.9211799	-1.69	*0.00*	-2.64
		HF	HF HF	11.8	-835.2865358	-1.76	*0.00*	-2.44
		HFHF	HF HF	13.6	-935.6465591	-3.25	*0.00*	-1.71
		HFHF	–	10.8	-734.9202784	-3.05	*0.00*	1.53
		HFHF	HF	13.3	-835.2846949	-2.92	*0.00*	0.57
		–	urea	11.6	-759.1334006	-3.52	*0.00*	-1.85
		–	4 H_2O	5.3	-839.5804997	-6.41 [b]	*0.00*	-2.89
	α	–	–	10.1	-534.1898574	*0.00*	1.69	2.60
		–	HF HF	15.6	-734.9184914	*0.00*	1.69	-0.95
		HF	HF HF	17.1	-835.2837241	*0.00*	1.76	-0.67
		HFHF	HF HF	18.9	-935.6413852	*0.00*	3.25	1.53
		HFHF	–	15.0	-734.9154225	*0.00*	3.05	4.58
		HFHF	HF	17.6	-835.2800353	*0.00*	2.92	3.49
		–	urea	14.0	-759.1277834	*0.00*	3.52	1.68
		–	4 H_2O	11.3	-839.5702832	*0.00*	6.41 [b]	3.53
	β	–	–	4.1	-534.1939966	-2.60	-0.91	*0.00*
		–	HF HF[c]	7.6	-734.9169770	0.95	2.64	*0.00*
		HF	HF HF[c]	9.0	-835.2826492	0.67	2.44	*0.00*
		HFHF	HF HF	6.8	-935.6438262	-1.53	1.71	*0.00*
		HFHF	–	8.1	-734.9227196	-4.58	-1.53	*0.00*
		HFHF	HF	5.2	-835.2855989	-3.49	-0.57	*0.00*
		–	urea	6.4	-759.1304564	-1.68	1.85	*0.00*
		–	4 H_2O	7.5	-839.5759012	-3.53 [b]	2.89	*0.00*

[a] Relative energies (E_{rel}) are referenced (italics) to the energy of the structure with the conformation indicated in column header and the given solvation pattern. All structures have *trans* Ac-Ala amide bonds.

[b] The 4-H_2O-cluster structure with an α-helix conformation contains one less H_2O-H_2O hydrogen bond than the H_2O-cluster structures with a PPII conformation or with a β conformation. A H_2O-H_2O hydrogen bond in water is favorable by 4.0 kcal mol^{-1} at this level of theory (Table S2). Thus, these numbers should properly be scaled to be 4.0 kcal mol^{-1} more favorable for the α-helix conformation than is indicated by the numbers in this table, in order to account for the differences in the number of H_2O-H_2O hydrogen bonds in the structures. Thus, the corrected values for the 4-H_2O clusters are that the PPII conformation is more stable than the α-helix conformation by 2.4 kcal mol^{-1} (instead of 6.4 kcal mol^{-1}), and the α-helix conformation is more stable than the β conformation by 0.5 kcal mol^{-1} (instead of the β conformation being more stable than the α-helix conformation by 3.5 kcal mol^{-1}).

[c] Attempts to achieve geometry optimization of this solvation pattern in a β conformation led to a change in conformation to PPII. In order to understand the energetics, these structures were

examined via geometry optimization with ϕ fixed at –160˚, as is present in the structure with implicit solvation. Torsion angle scans from $\phi = -140^\circ$ to $\phi = -180^\circ$ confirmed that there was no energy minimum in this region for these structures. These structures, while not local energy minima, nonetheless exhibited zero imaginary (negative) frequencies.

Table S6. Energies of Ac-Pro_2-NMe_2 in a PPII conformation, as a function of ring pucker and explicit solvation. Structures of all molecules were generated via geometry optimization using the M06-2X method with the 6-311++G(2d,2p) basis set in implicit water. Energies were determined using the MP2 method with the 6-311++G(3d,3p) basis set in implicit water (IEFPCM).

	explicit C=O solvation			***E*, hartrees** P1-P2 ring pucker				E_{rel}[a], kcal mol^{-1} P1-P2 ring pucker			
name	**Ac**	**P1**	**P2**	***exo-exo***	***exo-endo***	***endo-exo***	***endo-endo***	***exo-exo***	***exo-endo***	***endo-exo***	***endo-endo***
0HF	–	–	–	-935.2209428	-935.2221080	-935.2219268	-935.2232140	+1.43	+0.69	+0.81	*0.00*[a]
2HF	–	–	HFHF	-1135.8859701	-1135.8849488	-1135.8872452	-1135.8854639	–0.32	+0.32	–1.12	*0.00*[a]
3HF	–	HF	HFHF	-1236.2209899	-1236.2197641	-1236.2220193	-1236.2199704	–0.64	+0.13	–1.29	*0.00*[a]
4HF	HF	HF	HFHF	-1336.5546556	-1336.5533056	-1336.5557615	-1336.5536817	–0.61	+0.24	–1.31	*0.00*[a]
5HF	HF	HFHF	HFHF	-1436.8826624	-1436.8821577	-1436.8824899	-1436.8820137	–0.41	–0.09	–0.30	*0.00*[a]
5aHF	HFHF	HF	HFHF	-1436.8831392	-1436.8810929	-1436.8857429	-1436.8831047	–0.01	+1.26	–1.66	*0.00*[a]
5bHF	HFHF	HFHF	HF	-1436.8817699	-1436.8815572	-1436.8832169	-1436.8830800	+0.82	+0.96	–0.09	*0.00*[a]
6HF	HFHF	HFHF	HFHF	-1537.2107822	-1537.2096616	-1537.2123801	-1537.2108376	+0.03	+0.68	–0.97	*0.00*[a]

[a] Relative energies (E_{rel}) for each solvation pattern are referenced to the peptide with an *endo* ring pucker on both prolines in that solvation pattern. All structures have *trans* Ac-Pro and Pro-Pro amide bonds.

Coordinates of geometry-optimized structures

Coordinates of small molecule structures

HF

optimized MP2/augccpVTZ/H2O

0 1
F -0.00000000 0.00000000 0.09256827
H -0.00000000 -0.00000000 -0.83311447

1 2 1.0
2

H2O

optimized MP2/augccpVTZ/H2O

0 1
O -0.00000015 0.11883742 0.00000000
H 0.75740388 -0.47534867 0.00000000
H -0.75740265 -0.47535066 -0.00000000

1 2 1.0 3 1.0
2
3

HCHO

optimized MP2/augccpVTZ/H2O

0 1
C 0.00000696 0.53694166 0.00000000
H 0.93505350 1.11026527 0.00000000
H -0.93515092 1.11009971 0.00000000
O 0.00000696 -0.68025187 0.00000000

1 2 1.0 3 1.0 4 2.0
2
3
4

urea

optimized MP2/augccpVTZ/H2O

0 1
C 0.00000094 0.13129430 -0.00094879
O 0.00000139 1.36533844 0.01252318
N 1.15571370 -0.59815379 -0.05745486
H 1.99580168 -0.09403886 0.16901599
H 1.14529395 -1.57413117 0.18592710
N -1.15571756 -0.59815467 -0.05746824
H -1.99579238 -0.09403059 0.16903575
H -1.14529302 -1.57411342 0.18599017

1 2 2.0 3 1.0 6 1.0
2
3 4 1.0 5 1.0

4
5
6 7 1.0 8 1.0
7
8

thiourea

optimized MP2/augccpVTZ/H2O

0 1

C	-0.33408751	-0.00000086	-0.00014493
N	-1.03778208	-1.14092044	-0.00005051
H	-0.54001930	-2.01270934	0.00034508
H	-2.04426919	-1.15350455	0.00018505
N	-1.03777410	1.14092229	-0.00003097
H	-0.54000990	2.01271092	0.00016474
H	-2.04426715	1.15352212	0.00036444
S	1.35637399	-0.00000168	0.00002379

1 2 1.0 5 1.0 8 2.0
2 3 1.0 4 1.0
3
4
5 6 1.0 7 1.0
6
7
8

The above structure had one negative/imaginary frequency, even after multiple attempts at geometry optimization.

guanidinium

MP2/augccpVTZ/H2O optimized

1 1

C	0.00004471	0.00010977	0.00009161
N	-1.05771229	0.80357690	-0.00053959
H	-1.99042560	0.42997393	0.00724719
H	-0.94826173	1.80232871	-0.00275339
N	1.22489265	0.51403868	0.00123623
H	2.03488424	-0.08056213	-0.00774860
H	1.36812965	1.50852639	0.00287281
N	-0.16716597	-1.31769517	-0.00463409
H	0.62226417	-1.93855679	0.01910394
H	-1.08695973	-1.72181158	0.00829056

1 2 1.5 5 1.5 8 1.5
2 3 1.0 4 1.0
3
4
5 6 1.0 7 1.0
6
7
8 9 1.0 10 1.0
9
10

The above structure had one negative/imaginary frequency.

2H2O-lowD

optimized MP2/augccpVTZ/H2O **low dipole moment water dimer**

0 1 0 1 0 1

O(Fragment=1)	-1.48837400	0.01691800	-0.11786700
H(Fragment=1)	-0.51993400	0.00333400	-0.02321200
H(Fragment=1)	-1.81612400	-0.11388600	0.77699100
O(Fragment=2)	1.33332900	-0.01108100	0.09417500
H(Fragment=2)	1.78797200	-0.72355500	-0.36873900
H(Fragment=2)	1.78844300	0.78741200	-0.19549600

1 2 1.0 3 1.0
2
3
4 5 1.0 6 1.0
5
6

2H2O

optimized MP2/augccpVTZ/H2O **high dipole moment water dimer**

0 1 0 1 0 1

O(Fragment=1)	1.48972316	0.00287331	-0.09868670
H(Fragment=1)	0.51962920	0.00015345	-0.01900220
H(Fragment=1)	1.80270152	-0.02312689	0.81065475
O(Fragment=2)	-1.33575070	0.00169396	-0.07909368
H(Fragment=2)	-1.77795235	-0.76701856	0.29795326
H(Fragment=2)	-1.77615805	0.75345387	0.33263726

1 2 1.0 3 1.0
2
3
4 5 1.0 6 1.0
5
6

HCHO-HF

optimized MP2/augccpVTZ/H2O

0 1

C	-1.47367801	0.32540867	0.00000033
H	-1.20088174	1.38434613	-0.00000227
H	-2.53469381	0.06626283	0.00000212
O	-0.62141784	-0.55098683	-0.00000180
F	1.84709457	0.12520750	-0.00000182
H	0.92513522	-0.12203376	0.00002895

1 2 1.0 3 1.0 4 2.0
2
3
4
5 6 1.0
6

HCHO-HFHF

optimized MP2/augccpVTZ/H2O

```
0 1
 C              0.00011278    1.63112435    0.00111470
 H              0.93965208    2.18479718    0.00294257
 H             -0.93931409    2.18498679    0.00307600
 O             -0.00000788    0.40457843   -0.00326724
 F              2.26188042   -0.91761984    0.00088439
 H              1.44694167   -0.43856201   -0.00121952
 F             -2.26197729   -0.91750425    0.00087710
 H             -1.44702148   -0.43847880   -0.00120274

 1 2 1.0 3 1.0 4 2.0
 2
 3
 4
 5 6 1.0
 6
 7 8 1.0
 8
```

HCHO-HFHFHF

MP2/augccpVTZ/H2O optimized

```
0 1
 C              0.19273109   -1.25461890    1.39258883
 H              1.15608350   -1.38264566    1.88704291
 H             -0.70424195   -1.64888255    1.87105939
 O              0.11872054   -0.67494037    0.31152479
 F              2.36558402   -0.07730106   -0.96591405
 H              1.56774293   -0.28872614   -0.51181614
 F             -2.18485254   -0.73551920   -1.00084062
 H             -1.36748273   -0.71113811   -0.53295310
 F             -0.45868454    2.51772372    0.41232107
 H             -0.25667510    1.61449769    0.42883802

 1 2 1.0 3 1.0 4 2.0
 2
 3
 4
 5 6 1.0
 6
 7 8 1.0
 8
 9 10 1.0
 10
```

This structure had one negative/imaginary frequency. Energy analysis of this structure (Table S2) indicates no additional hydrogen bonding energy (beyond the structure with 2 HF bound), despite one additional hydrogen bond donor.

HCHO-4HF

MP2/augccpVTZ/H2O optimized model 60 (lowest E/error)

```
0 1
 C(Iso=12)        -0.45230033    0.01451030    1.99750325
 H(Iso=1)         -0.50735105    0.95713446    2.54285696
 H(Iso=1)         -0.49673708   -0.92251671    2.55331618
 O(Iso=16)        -0.34237420    0.00839879    0.77354336
 F(Iso=19)         0.10847765    2.29148964   -0.49098568
 H(Iso=1)         -0.05954286    1.48250273   -0.03766607
 F(Iso=19)         0.12956004   -2.28307056   -0.46612153
 H(Iso=1)         -0.04676525   -1.47123633   -0.02107416
 F(Iso=19)        -3.16879037   -0.02541397   -1.00054911
 H(Iso=1)         -2.42569073   -0.00090643   -0.44939806
 F(Iso=19)         3.61807133   -0.00860069   -0.55793576
 H(Iso=1)          2.80301472    0.03113047   -0.12107262

 1 2 1.0 3 1.0 4 2.0
 2
 3
 4
 5 6 1.0
 6
 7 8 1.0
 8
 9 10 1.0
 10
 11 12 1.0
 12
```

This structure did not optimize to a stable energy minimum (no convergence). Energy analysis of this structure (Table S2) indicates no additional hydrogen bonding energy (beyond the structures with 2 HF bound or with 3 HF bound), despite one or two additional hydrogen bond donors.

HCHO-H2O

optimized MP2/augccpVTZ/H2O

```
0 1
 C              -1.56417953    0.35362370   -0.00130808
 H              -1.22649064    1.39567948   -0.02126775
 H              -2.64372097    0.17179156    0.00335298
 O              -0.76922185   -0.57135218    0.01507387
 O               2.00432571    0.09849364   -0.10942008
 H               2.30790001    0.23327538    0.79372860
 H               1.06655789   -0.13962029   -0.01319570

 1 2 1.0 3 1.0 4 2.0
 2
 3
 4
 5 6 1.0 7 1.0
 6
 7
```

HCHO-H2OH2O

optimized MP2/augccpVTZ/H2O

```
0 1
 C              0.00000266   1.66801193   0.00893169
 H              0.93746362   2.23165873   0.01214535
 H             -0.93744865   2.23167731   0.01215361
 O              0.00000117   0.44605887   0.00186548
 O              2.52980829  -0.93350062  -0.10434307
 H              2.81916007  -1.07262138   0.80290850
 H              1.67666961  -0.47934133  -0.01459585
 O             -2.52983146  -0.93345984  -0.10433826
 H             -2.81901190  -1.07289383   0.80291977
 H             -1.67667271  -0.47933835  -0.01459477

 1 2 1.0 3 1.0 4 2.0
 2
 3
 4
 5 6 1.0 7 1.0
 6
 7
 8 9 1.0 10 1.0
 9
 10
```

HCHO-urea

optimized MP2/augccpVTZ/H2O

```
0 1
 C              3.23231306  -0.00101273  -0.02859202
 H              3.80118232   0.93443465  -0.00804218
 H              3.79661440  -0.93917702  -0.00583361
 O              2.01398375   0.00190707  -0.07740820
 C             -1.47968996  -0.00025363   0.01226061
 O             -2.70550613  -0.00112497  -0.14925449
 N             -0.75692462  -1.15203228   0.14994368
 H             -1.22895734  -1.99601226  -0.12443817
 H              0.24503908  -1.12196602   0.03699207
 N             -0.75862591   1.15261773   0.15007505
 H             -1.23192200   1.99586180  -0.12440514
 H              0.24333764   1.12410207   0.03688594

 1 2 1.0 3 1.0 4 2.0
 2
 3
 4
 5 6 2.0 7 1.0 10 1.0
 6
 7 8 1.0 9 1.0
 8
 9
 10 11 1.0 12 1.0
 11
 12
```

HCHO-thiourea

optimized MP2/augccpVTZ/H2O

0 1

C	-3.71495057	-0.00015304	0.03194890
H	-4.27985233	-0.93720434	0.06363975
H	-4.28048806	0.93661809	0.06039240
O	-2.49692033	0.00014967	-0.03373632
C	0.93619726	0.00003763	-0.00476783
N	0.23029176	1.13918585	-0.01318397
H	0.72767019	2.01105421	-0.00695645
H	-0.78033135	1.13067155	-0.02428398
N	0.23004593	-1.13894949	-0.01352129
H	0.72722768	-2.01092977	-0.00726449
H	-0.78058536	-1.13017646	-0.02420205
S	2.63074237	-0.00013705	0.01452599

1 2 1.0 3 1.0 4 2.0
2
3
4
5 6 1.0 9 1.0 12 2.0
6 7 1.0 8 1.0
7
8
9 10 1.0 11 1.0
10
11
12

HCHO-guanidinium

optimized MP2/augccpVTZ/H2O

1 1

C	-3.23011900	0.00005800	0.08240000
H	-3.78998500	0.93735900	0.15278900
H	-3.79021300	-0.93710000	0.15289000
O	-2.01930100	-0.00009800	-0.06985300
C	1.30936500	0.00000400	-0.00770200
N	0.64128900	-1.14725000	-0.04980900
H	1.12638200	-2.02637300	-0.02317100
H	-0.36791200	-1.13462900	-0.09529100
N	0.64122100	1.14722000	-0.04981900
H	1.12625800	2.02637000	-0.02309000
H	-0.36798100	1.13453300	-0.09526300
N	2.63897000	0.00004500	0.05877700
H	3.14598700	0.86113800	0.16374700
H	3.14604100	-0.86098800	0.16398100

1 2 1.0 3 1.0 4 2.0
2
3
4
5 6 1.5 9 1.5 12 1.5
6 7 1.0 8 1.0
7
8
9 10 1.0 11 1.0
10
11
12 13 1.0 14 1.0
13
14

HCHO-Hacceptor

MP2/aug-cc-pVTZ/H2O optimized

1 1
C -0.62402592 0.03243198 0.00001290
H -1.05773333 1.02479938 -0.00002249
H -1.21931066 -0.86990844 -0.00003613
O 0.61272359 -0.13221203 -0.00000036
H 1.11941073 0.70821337 -0.00001592

1 2 1.0 3 1.0 4 2.0
2
3
4
5

HCHO-Liacceptor

MP2/augccpVTZ/H2O optimized

1 1
C 0.84221342 0.22383942 -0.00000014
H 0.80950381 1.31752573 0.00001866
H 1.82442969 -0.25601924 0.00002252
O -0.18067232 -0.44300733 -0.00001414
Li -2.08061180 0.37983855 0.00002426

1 2 1.0 3 1.0 4 2.0
2
3
4
5

HCHO-Naacceptor

MP2/augccpVTZ/H2O optimized

1 1
C 1.73892813 0.19715007 -0.00006349
H 1.81754573 1.28933530 -0.00009304
H 2.67121370 -0.37686952 0.00012466
O 0.65530881 -0.36341848 -0.00000663
Na -1.83316352 0.07381651 0.00003658

1 2 1.0 3 1.0 4 2.0
2
3
4
5

HCHO-Kacceptor

MP2/augccpVTZ-6311pp3d3p/H2O optimized

```
1 1
 C              -2.28332748    0.35402501    0.00001266
 H              -1.94749219    1.39886767    0.00001168
 H              -3.36649533    0.17500982   -0.00001206
 O              -1.48906298   -0.56881355    0.00005208
 K               1.62770822    0.04486741   -0.00002591

 1 2 1.0 3 1.0 4 2.0
 2
 3
 4
 5
```

2HCHO

MP2/augccpVTZ/H2O optimized

```
0 1 0 1 0 1
 C(Fragment=1)    -2.12014561    0.25537301   -0.00005867
 H(Fragment=1)    -1.85875180    1.32139995    0.00031974
 H(Fragment=1)    -3.18744416    0.00444961   -0.00046128
 O(Fragment=1)    -1.26269203   -0.60915732   -0.00003270
 C(Fragment=2)     1.34949362    0.49246868    0.00011593
 H(Fragment=2)     0.93606798    0.89139635   -0.93375142
 H(Fragment=2)     0.93619903    0.89117964    0.93413528
 O(Fragment=2)     2.23742214   -0.34027714   -0.00004053

 1 2 1.0 3 1.0 4 2.0
 2
 3
 4
 5 6 1.0 7 1.0 8 2.0
 6
 7
 8
```

2HCHO-HFdonor

optimized MP2/aug-cc-pvtz/H2O v3

```
0 1 0 1 0 1
 C(Fragment=1)    -1.14217543    1.65342887   -0.01991710
 H(Fragment=1)    -0.47169554    2.51616150   -0.02596607
 H(Fragment=1)    -2.21993759    1.83671260   -0.02674095
 O(Fragment=1)    -0.68967256    0.51749408   -0.00574093
 C(Fragment=2)     2.17936001    0.23703829    0.05761842
 H(Fragment=2)     2.04545442    0.88589365   -0.81634033
 H(Fragment=2)     1.97792576    0.68159525    1.03959420
 O(Fragment=2)     2.54521191   -0.91817892   -0.05647646
 F(Fragment=1)    -2.29921240   -1.48041816    0.01075562
 H(Fragment=1)    -1.70625765   -0.73392368    0.00418372

 1 2 1.0 3 1.0 4 2.0
 2
 3
 4
 5 6 1.0 7 1.0 8 2.0
 6
 7
 8
 9 10 1.0
 10
```

2HCHO-HFacceptor

optimized MP2/augccpVTZ/H2O v2

0 1 0 1 0 1

C(Fragment=1)	2.84550646	-0.39277695	0.20883440
H(Fragment=1)	2.94118574	0.28000740	1.07010765
H(Fragment=1)	3.71868109	-1.00286894	-0.04899496
O(Fragment=1)	1.81251472	-0.45877022	-0.43381198
C(Fragment=2)	-0.24798130	1.07229794	0.32570789
H(Fragment=2)	-0.11853036	0.48198493	1.23600465
H(Fragment=2)	0.47625207	1.86249976	0.12065717
O(Fragment=2)	-1.19150341	0.88206602	-0.42927153
F(Fragment=2)	-2.81870482	-0.97864249	0.15362220
H(Fragment=2)	-2.20248660	-0.27733313	-0.06295999

1 2 1.0 3 1.0 4 2.0
2
3
4
5 6 1.0 7 1.0 8 2.0
6
7
8
9 10 1.0
10

2HCHO-HFdonor-HFacceptor

optimized MP2/augccpVTZ/H2O

0 1 0 1 0 1

C(Fragment=1)	-2.74526397	-0.56358614	0.42830833
H(Fragment=1)	-3.03113981	-1.58805699	0.67639403
H(Fragment=1)	-3.51622112	0.21096295	0.45527595
O(Fragment=1)	-1.58951602	-0.29817587	0.12864488
C(Fragment=2)	0.78562010	-1.65046569	-0.15363773
H(Fragment=2)	0.71697883	-1.66628660	0.93693764
H(Fragment=2)	0.19904848	-2.38086298	-0.71437279
O(Fragment=2)	1.50636840	-0.85264045	-0.73594106
F(Fragment=2)	2.79193781	0.83165872	0.67676845
H(Fragment=2)	2.30986956	0.19684503	0.14722926
F(Fragment=1)	-0.91209134	2.11219975	-0.46020033
H(Fragment=1)	-1.17411003	1.22351392	-0.24023126

1 2 1.0 3 1.0 4 2.0
2
3
4
5 6 1.0 7 1.0 8 2.0
6
7
8
9 10 1.0
10
11 12 1.0
12

2HCHO-HFHFacceptor

MP2/aug-cc-pVTZ/H2O optimized

0 1 0 1 0 1

C(Fragment=1)	3.22099669	-0.00036946	-0.15110211
H(Fragment=1)	3.44558710	0.00171616	0.92224502
H(Fragment=1)	4.07050215	-0.00176906	-0.84263412
O(Fragment=1)	2.07236220	-0.00110618	-0.55981199
C(Fragment=2)	0.10131924	0.00025249	1.05887086
H(Fragment=2)	0.54652180	-0.93685814	1.39078810
H(Fragment=2)	0.54697235	0.93753443	1.38969999
O(Fragment=2)	-0.91472997	0.00009109	0.36850209
F(Fragment=2)	-1.92815065	-2.27074742	-0.36536487
H(Fragment=2)	-1.55838085	-1.43883108	-0.09817666
F(Fragment=2)	-1.92616462	2.27160883	-0.36570034
H(Fragment=2)	-1.55731849	1.43927750	-0.09846887

1 2 1.0 3 1.0 4 2.0
2
3
4
5 6 1.0 7 1.0 8 2.0
6
7
8
9 10 1.0
10
11 12 1.0
12

2HCHO-3HF

optimized MP2/augccpVTZ/H2O **HF donor HFHF acceptor**

0 1 0 1 0 1

C(Fragment=1)	3.06565065	-0.00009210	-0.62364824
H(Fragment=1)	3.37068075	-0.00031495	-1.67215128
H(Fragment=1)	3.84349682	0.00002734	0.14409795
O(Fragment=1)	1.87972312	0.00002174	-0.32310610
C(Fragment=2)	-0.44548362	-0.00027741	-1.60759596
H(Fragment=2)	-0.09688064	0.93751829	-2.03988241
H(Fragment=2)	-0.09674091	-0.93816375	-2.03957349
O(Fragment=2)	-1.23408567	-0.00017815	-0.66730380
F(Fragment=2)	-1.99147576	2.26913341	0.36052181
H(Fragment=2)	-1.71952213	1.44292127	-0.01463937
F(Fragment=2)	-1.99120009	-2.26915291	0.36123149
H(Fragment=2)	-1.71931539	-1.44302909	-0.01420327
F(Fragment=1)	1.10708378	0.00048457	2.13522237
H(Fragment=1)	1.41250826	0.00032357	1.23431522

1 2 1.0 3 1.0 4 2.0
2
3
4
5 6 1.0 7 1.0 8 2.0
6
7
8
9 10 1.0
10
11 12 1.0
12
13 14 1.0
14

2HCHO-H2Odonor

MP2/augcccpVTZ/H2O optimized

0 1 0 1 0 1

C(Fragment=1)	-0.91119364	1.79875080	0.01027726
H(Fragment=1)	-0.16942543	2.60466835	0.01208147
H(Fragment=1)	-1.96895846	2.08287699	0.01638127
O(Fragment=1)	-0.56747752	0.62806722	0.00159688
C(Fragment=2)	2.22664084	0.09475510	-0.00698395
H(Fragment=2)	2.10911207	0.64610454	-0.94741925
H(Fragment=2)	2.12014692	0.67037825	0.92017263
O(Fragment=2)	2.47797655	-1.09621247	0.00709508
O(Fragment=1)	-2.58016602	-1.39979259	-0.10821379
H(Fragment=1)	-2.73632019	-1.69994926	0.79266236
H(Fragment=1)	-1.88990227	-0.72161155	-0.01746378

1 2 1.0 3 1.0 4 2.0
2
3
4
5 6 1.0 7 1.0 8 2.0
6
7
8
9 10 1.0 11 1.0
10
11

2HCHO-H2Oacceptor

2 HCHO H2O acceptor MP2/augccpVTZ/H2O optimized v2

0 1 0 1 0 1

C(Fragment=1)	2.88569794	-0.46868436	0.23259616
H(Fragment=1)	2.94660860	0.17875144	1.11648759
H(Fragment=1)	3.76340517	-1.08429118	0.00358832
O(Fragment=1)	1.88660720	-0.50138199	-0.46323285
C(Fragment=2)	-0.18928970	1.12694294	0.34363261
H(Fragment=2)	-0.10358547	0.46355706	1.21057851
H(Fragment=2)	0.59317529	1.87971361	0.20792206
O(Fragment=2)	-1.13084359	1.04779089	-0.42833316
O(Fragment=2)	-2.92902546	-1.08710948	0.07406220
H(Fragment=2)	-3.63760167	-0.74435105	0.62758230
H(Fragment=2)	-2.35435655	-0.31732679	-0.08350089

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9 10 1.0 11 1.0
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2HCHO-H2OH2Oacceptor

MP2/augccpVTZ/H2O optimized

0 1 0 1 0 1

C(Fragment=1)	3.29332531	-0.00009980	-0.11383162
H(Fragment=1)	3.44844728	-0.00133429	0.97220565
H(Fragment=1)	4.18798005	0.00064284	-0.74697304
O(Fragment=1)	2.17423384	0.00042237	-0.59540940
C(Fragment=2)	0.07413121	-0.00000433	1.07465504
H(Fragment=2)	0.54015034	-0.93565487	1.39464749
H(Fragment=2)	0.53998928	0.93568909	1.39475217
O(Fragment=2)	-0.95030517	-0.00005247	0.40720927
O(Fragment=2)	-1.89186158	-2.55934914	-0.45609580
H(Fragment=2)	-2.59700411	-2.82742253	0.14144008
H(Fragment=2)	-1.62309490	-1.68413493	-0.13024218
O(Fragment=2)	-1.89219548	2.55914852	-0.45602821
H(Fragment=2)	-2.59686272	2.82749756	0.14194475
H(Fragment=2)	-1.62331727	1.68398769	-0.13012231

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12 13 1.0 14 1.0
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2HCHO-H2Odonor-H2Oacceptor

MP2/augccpVTZ/H2O optimized

0 1 0 1 0 1

C(Fragment=1)	-2.84513362	-0.31262262	0.64447770
H(Fragment=1)	-3.29997011	-1.24743637	0.98731848
H(Fragment=1)	-3.44482637	0.60088982	0.71877583
O(Fragment=1)	-1.71046194	-0.29197470	0.19614656
C(Fragment=2)	0.58881699	-1.73161182	-0.36621202
H(Fragment=2)	0.55549145	-1.86996319	0.71953798
H(Fragment=2)	-0.07625345	-2.35459475	-0.97219853
O(Fragment=2)	1.34351972	-0.92419110	-0.88255416
O(Fragment=2)	2.76055264	0.69999547	0.96564722
H(Fragment=2)	3.57280731	0.23305836	1.18561097
H(Fragment=2)	2.32282033	0.12363425	0.31471099
H(Fragment=1)	-0.89300339	1.31675952	-0.40346518
O(Fragment=1)	-0.41244485	2.09715823	-0.72597964
H(Fragment=1)	-1.04849055	2.81515583	-0.64596447

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9 10 1.0 11 1.0
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12 13 1.0
13 14 1.0
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2HCHO-HFdonor-H2OH2Oacceptor

MP2/augccpVTZ/H2O optimized

0 1 0 1 0 1

C(Fragment=1)	3.10954052	0.03503373	-0.37641883
H(Fragment=1)	3.61055988	0.00616759	-1.34639151
H(Fragment=1)	3.72724123	0.05620092	0.52530448
O(Fragment=1)	1.88824323	0.04332217	-0.30964607
C(Fragment=2)	-0.47783286	-0.04529076	-1.73966081
H(Fragment=2)	-0.15507711	0.89275134	-2.20002846
H(Fragment=2)	-0.09327760	-0.97830165	-2.16106788
O(Fragment=2)	-1.24979987	-0.05107998	-0.79238115
O(Fragment=2)	-1.81260098	2.48393070	0.41984746
H(Fragment=2)	-2.59312362	2.85516999	-0.00349841
H(Fragment=2)	-1.69038472	1.62523680	-0.01741700
O(Fragment=2)	-1.61988578	-2.57196940	0.51891607
H(Fragment=2)	-2.39337754	-2.99991097	0.13828991
H(Fragment=2)	-1.56476597	-1.72164912	0.05259224
F(Fragment=1)	0.72816144	0.11178057	1.98627503
H(Fragment=1)	1.16085368	0.08622422	1.13832870

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5 6 1.0 7 1.0 8 2.0
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9 10 1.0 11 1.0
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12 13 1.0 14 1.0
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15 16 1.0
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2HCHO-H2Odonor-H2OH2Oacceptor

MP2/augccpVTZ/H2O optimized

0 1 0 1 0 1

C(Fragment=1)	3.20188786	-0.00002370	-0.35665181
H(Fragment=1)	3.71337209	0.00036033	-1.32441588
H(Fragment=1)	3.82185659	0.00073047	0.54603505
O(Fragment=1)	1.98344359	-0.00125595	-0.28881897
C(Fragment=2)	-0.33508188	0.00021491	-1.69607945
H(Fragment=2)	0.04459773	0.93586175	-2.11551252
H(Fragment=2)	0.04373120	-0.93569239	-2.11570152
O(Fragment=2)	-1.16488131	0.00048692	-0.79868399
O(Fragment=2)	-1.78911979	2.55649757	0.33002397
H(Fragment=2)	-2.49339037	2.94003405	-0.20213430
H(Fragment=2)	-1.63272825	1.68650332	-0.07364962
O(Fragment=2)	-1.79124736	-2.55521295	0.32912662

H(Fragment=2)	-2.49595930	-2.93774400	-0.20317228
H(Fragment=2)	-1.63402197	-1.68514762	-0.07409787
H(Fragment=1)	1.00428800	-0.00126469	1.34933150
O(Fragment=1)	0.43378563	-0.00083785	2.13535690
H(Fragment=1)	1.05157223	-0.00221049	2.87366875

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9 10 1.0 11 1.0
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12 13 1.0 14 1.0
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15 16 1.0
16 17 1.0
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2HCHO-urea

optimized MP2/augccpVTZ/H2O

0 1 0 1 0 1

C(Fragment=1)	-4.52449411	-0.65478658	0.00032521
H(Fragment=1)	-4.91159197	0.37197108	-0.00264526
H(Fragment=1)	-5.26166172	-1.46616013	0.00245055
O(Fragment=1)	-3.32792792	-0.88239806	0.00120646
C(Fragment=2)	-1.70354246	1.32530890	-0.00154133
H(Fragment=2)	-2.24554629	1.49461930	-0.93725830
H(Fragment=2)	-2.24690661	1.49768632	0.93286060
O(Fragment=2)	-0.53285767	0.98358822	-0.00010892
C(Fragment=2)	2.72143737	-0.24162258	0.00004307
O(Fragment=2)	3.93239193	-0.49270407	-0.00026430
N(Fragment=2)	1.99405090	-0.13314803	1.15194729
H(Fragment=2)	2.52943787	-0.02778510	1.99612001
H(Fragment=2)	1.08397876	0.30172469	1.11873271
N(Fragment=2)	1.99292648	-0.13546283	-1.15130193
H(Fragment=2)	2.52734298	-0.03246652	-1.99637082
H(Fragment=2)	1.08284982	0.29939923	-1.11803479

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9 10 2.0 11 1.5 14 1.5
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11 12 1.0 13 1.0
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14 15 1.0 16 1.0
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2HCHO-thiourea

optimized MP2/augccpVTZ/H2O

0 1 0 1 0 1

C(Fragment=1)	-5.00459147	-0.79102332	-0.00459119
H(Fragment=1)	-5.43015176	0.22037998	-0.01750536
H(Fragment=1)	-5.71037810	-1.62972792	-0.00282328
O(Fragment=1)	-3.80023997	-0.97318856	0.00732121
C(Fragment=2)	-2.27428546	1.28645559	0.00001451
H(Fragment=2)	-2.82332083	1.42946781	-0.93543348
H(Fragment=2)	-2.82216857	1.43502487	0.93525321
O(Fragment=2)	-1.08837238	0.99944854	0.00014095
C(Fragment=2)	2.17031478	-0.01587781	-0.00022813
N(Fragment=2)	1.49651104	0.19679401	1.13844132
H(Fragment=2)	1.97028909	0.04832904	2.01078632
H(Fragment=2)	0.53123707	0.49812620	1.12608988
N(Fragment=2)	1.49543516	0.19508789	-1.13856940
H(Fragment=2)	1.96816685	0.04460793	-2.01113625
H(Fragment=2)	0.53007550	0.49615878	-1.12570455
S(Fragment=2)	3.78768120	-0.52330916	-0.00059365

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13 14 1.0 15 1.0
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2HCHO-guanidinium

optimized MP2/augccpVTZ/H2O

1 1

C	4.58856579	-0.63771016	-0.00236654
H	4.96994413	0.39075836	0.02186050
H	5.32949251	-1.44534747	-0.01277516
O	3.39304841	-0.87163956	-0.01719523
C	1.73476654	1.25752028	0.01444805
H	2.26698876	1.43373255	0.95310844
H	2.26802781	1.46181382	-0.91786324
O	0.57542522	0.87480313	0.00805966
C	-2.56458763	-0.17065033	-0.00127246
N	-1.92773674	0.04574134	-1.14706198
H	-2.38999324	-0.09335816	-2.02810673
H	-0.96626428	0.35784659	-1.12811381
N	-1.92237626	0.01708919	1.14646288
H	-2.38342455	-0.13520258	2.02593217
H	-0.96085960	0.32950745	1.13076152
N	-3.83219260	-0.57536942	-0.00344177
H	-4.32670983	-0.72856800	0.85722771
H	-4.33131977	-0.70367757	-0.86551509

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5 6 1.0 7 1.0 8 2.0
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9 10 1.5 13 1.5 16 1.5
10 11 1.0 12 1.0
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13 14 1.0 15 1.0
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16 17 1.0 18 1.0
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The above structure had one negative/imaginary frequency.

2HCHO-Hacceptor

2 HCHO H+ acceptor MP2/augccpVTZ/H2O optimized

1 1

C	1.69336256	0.03188241	-0.22274492
H	1.72099566	0.99334734	-0.72923833
H	2.56530593	-0.60778909	-0.15795756
O	0.65499621	-0.38038806	0.31322429
C	-0.63938367	0.49958767	0.24343089
H	-0.79561544	0.71158833	1.29488227
H	-0.35070024	1.35624916	-0.35543888
O	-1.58261830	-0.22606953	-0.36875987
H	-2.04288249	-0.79055553	0.26792122

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2HCHO-Liacceptor

MP2/augccpVTZ/H2O optimized

1 1

C	-2.38962737	-0.00846576	0.14116709
H	-2.36510816	-1.00351365	0.60265795
H	-3.36902111	0.47440027	0.04608271
O	-1.37192439	0.53610575	-0.24824384
C	0.96935565	-0.77758511	0.15127220
H	0.64628360	-0.62861975	1.18502376
H	0.45349774	-1.54269102	-0.43431408
O	1.89011231	-0.13711408	-0.33005547
Li	3.00349162	1.40826532	0.49076947

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2HCHO-Naacceptor

MP2/augccpVTZ/H2O optimized

1 1

C	3.02270816	-0.38392012	0.21886214
H	3.11040789	0.42599014	0.95406504
H	3.90939244	-1.00730030	0.05494352
O	1.98528773	-0.58115151	-0.38808798
C	-0.08345321	1.13850324	0.22794044
H	0.13279629	0.71473906	1.21367444
H	0.63814956	1.85280746	-0.17998930
O	-1.09863347	0.84691982	-0.38393320
Na	-2.95631909	-0.78544378	0.13206002

1 2 1.0 3 1.0 4 2.0
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5 6 1.0 7 1.0 8 2.0
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2HCHO-Kacceptor

MP2/augccpVTZ-6311pp3d3p/H2O optimized

1 1 0 1 1 1

C(Fragment=1)	3.61145868	-0.55478598	0.09208329
H(Fragment=1)	3.89492297	0.41560556	0.51939928
H(Fragment=1)	4.41087403	-1.29328376	-0.04058871
O(Fragment=1)	2.46016543	-0.79970983	-0.22067599
C(Fragment=2)	0.66170827	1.25075631	0.32652322
H(Fragment=2)	0.63200645	0.70048128	1.27489530
H(Fragment=2)	1.56964343	1.83104761	0.11509279
O(Fragment=2)	-0.27630992	1.23577847	-0.44970856
K(Fragment=2)	-2.82196277	-0.49043273	0.05171783

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Coordinates of structures of Ac-Pro-NMe_2 as a function of ring pucker, main chain conformation, and explicit solvation

Ac-Pro-NMe2-endo-alpha-guanidinium

optimized M062X/junccpVTZ/H2O

1 1

N	-2.23975966	-0.66177969	0.27065752
O	-1.96894689	0.55080464	2.13892213
O	1.23475533	0.32224451	0.07113644
C	-3.02961658	-1.36141201	-0.74884696
C	-1.99576685	-1.69990981	-1.82201138
C	-0.69690326	-1.86443316	-1.03225961
C	-0.80898992	-0.82067961	0.09237325
C	-2.72497665	0.00596478	1.33749155
C	-4.22319101	0.07000274	1.46362619
C	0.02125424	0.43419021	-0.17784267
C	0.44481599	2.72067489	-0.69978965
H	-0.36935369	-1.19671857	1.01573722
H	-3.83242639	-0.72648732	-1.12244773
H	-3.47410339	-2.26528645	-0.32803992
H	0.19843295	-1.72449904	-1.63292053
H	-0.65362115	-2.85554815	-0.58325476
H	-4.47815883	0.51587899	2.41913397
H	-4.66888195	-0.92054208	1.38231196
H	-4.63366153	0.68332710	0.65944310
H	1.07585833	2.66302310	-1.58763506
H	1.07785399	2.73626308	0.18301348
H	-0.14198749	3.63349462	-0.73651048
H	-2.26595920	-2.59513402	-2.37533620
H	-1.90435556	-0.88270366	-2.53728961
N	-0.47164072	1.58381478	-0.63624594
C	-1.83257006	1.84098406	-1.09832435
H	-1.77814185	2.59207459	-1.88243321
H	-2.28875616	0.95679201	-1.52221146
H	-2.45479467	2.22467208	-0.28808165
C	4.38350746	-0.37153522	0.30074932
N	3.46918873	-1.26623691	0.64937500
H	3.73945440	-2.16154066	1.01656603
H	2.48718320	-1.01789344	0.56435223
N	3.99114990	0.81057025	-0.15599731
H	4.66122115	1.50206196	-0.44317888
H	2.99601087	1.00065655	-0.22607355
N	5.67858973	-0.65794477	0.40505229
H	6.38051769	0.01971760	0.16449399
H	5.98312558	-1.54804853	0.75900740

1 4 1.0 7 1.0 8 1.5
2 8 2.0
3 10 2.0
4 5 1.0 13 1.0 14 1.0
5 6 1.0 23 1.0 24 1.0
6 7 1.0 15 1.0 16 1.0
7 10 1.0 12 1.0
8 9 1.0
9 17 1.0 18 1.0 19 1.0
10 25 1.5
11 20 1.0 21 1.0 22 1.0 25 1.0
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26 27 1.0 28 1.0 29 1.0
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30 31 1.5 34 1.5 37 1.5
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37 38 1.0 39 1.0
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Ac-Pro-NMe2-endo-alpha-H2OcisHFtrans

optimized M062X/junccpVTZ/H2O

0 1

N	-1.62499096	0.38834121	-0.12312502
O	-1.40490203	-0.77102440	-2.03064185
O	1.96872302	0.10937233	-0.41505938
C	-2.37548440	0.94438827	1.00881002
C	-1.27816137	1.49727619	1.91788895
C	-0.16888075	1.89265199	0.94273103
C	-0.24098184	0.81606645	-0.15277340
C	-2.12802632	-0.36357322	-1.12488068
C	-3.59487199	-0.68886066	-1.04626647
C	0.83866596	-0.25300292	-0.00558008
C	1.74485468	-2.42949123	0.37958901
H	-0.01472025	1.24369574	-1.12966332
H	-2.97543684	0.17442803	1.49313156
H	-3.04408621	1.73633557	0.66675658
H	0.81594961	1.95088721	1.39949862
H	-0.38800753	2.85820856	0.48989598
H	-3.88953927	-1.21006731	-1.95080242
H	-4.18944100	0.21634608	-0.92700225
H	-3.78803941	-1.32669433	-0.18218078
H	1.32830557	-3.42926802	0.45266286
H	2.46750832	-2.27862032	1.18108737
H	2.24711267	-2.31880912	-0.57724140
H	-1.62973117	2.33479411	2.51407510
H	-0.92402150	0.72652176	2.60279861
N	0.64534280	-1.46860948	0.48018369
C	-0.56519359	-1.97003603	1.12901010
H	-0.25653452	-2.69204677	1.88060949
H	-1.10775018	-1.18108320	1.63107204
H	-1.21300289	-2.46778361	0.40656223
H	2.24055787	1.90533202	-0.87775397
O	2.31528343	2.85861679	-1.04648979
H	2.79082262	2.93223355	-1.87778306
F	4.28963207	-0.60865423	0.00971399
H	3.35654487	-0.38287476	-0.13620260

1 4 1.0 7 1.0 8 1.5
2 8 2.0
3 10 2.0
4 5 1.0 13 1.0 14 1.0
5 6 1.0 23 1.0 24 1.0

6 7 1.0 15 1.0 16 1.0
7 10 1.0 12 1.0
8 9 1.0
9 17 1.0 18 1.0 19 1.0
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30 31 1.0
31 32 1.0
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33 34 1.0
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Ac-Pro-NMe2-endo-alpha-H2Ocis

optimized M062X/junccpVTZ/H2O

0 1

N	1.14403841	-0.61498233	-0.11418050
O	1.20895538	0.49404208	-2.06512154
O	-2.31891635	0.44098548	-0.38785239
C	1.74585458	-1.27659359	1.04978507
C	0.54475945	-1.55216191	1.95304185
C	-0.60547845	-1.74438540	0.96479744
C	-0.30273790	-0.72739256	-0.14684089
C	1.81041402	-0.02915232	-1.12935936
C	3.31264245	-0.02875002	-1.03204392
C	-1.14095391	0.54961935	-0.01653160
C	-1.52714968	2.88747468	0.38644947
H	-0.61138602	-1.11188991	-1.11835974
H	2.49065262	-0.63549136	1.52128915
H	2.23451412	-2.20440441	0.74629969
H	-1.58938066	-1.59489386	1.40218020
H	-0.57172556	-2.74597259	0.53796439
H	3.72546305	0.37418162	-1.95076654
H	3.69554028	-1.03444234	-0.86198602
H	3.62939730	0.59105510	-0.19158206
H	-1.99525919	3.07025141	1.35492488
H	-2.29681253	2.74197486	-0.36194233
H	-0.91647139	3.74888089	0.12259407
H	0.70642642	-2.41855813	2.58865988
H	0.34757251	-0.69545846	2.59794554
N	-0.66605395	1.71076933	0.44809948
C	0.63886233	1.95403386	1.05231097
H	0.52157961	2.76489514	1.76794687
H	1.00197054	1.09121164	1.59396512
H	1.37230080	2.25641894	0.30244961
H	-2.96381725	-1.15595494	-0.85667339
O	-3.29060726	-2.05328214	-1.06406969
H	-3.77918740	-1.96242831	-1.88564748

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26 27 1.0 28 1.0 29 1.0
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30 31 1.0
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Ac-Pro-NMe2-endo-alpha-HFcis

optimized M062X/junccpVTZ/H2O

0 1

N	1.19919113	-0.50161181	-0.13583008
O	1.07762195	0.70495049	-2.02337233
O	-2.36336513	0.14086785	-0.38496004
C	1.90220933	-1.13842265	0.98360678
C	0.76481300	-1.59207372	1.89780404
C	-0.38455966	-1.87260333	0.92935438
C	-0.21989284	-0.79698436	-0.15906175
C	1.76419786	0.21542681	-1.12967421
C	3.25585147	0.39947074	-1.05644476
C	-1.19737835	0.36596899	0.01063840
C	-1.87939287	2.61610577	0.50535393
H	-0.48759732	-1.19403709	-1.13809122
H	2.57784112	-0.43461952	1.46891089
H	2.48804799	-1.98831932	0.62883602
H	-1.36590854	-1.83873585	1.39587539
H	-0.26059402	-2.85130371	0.46844651
H	3.59573331	0.89340166	-1.96047368
H	3.76256246	-0.55815239	-0.94182703
H	3.51169530	1.01327758	-0.19112154
H	-1.37210727	3.54818202	0.26472526
H	-2.35171529	2.71253456	1.48336451
H	-2.63396815	2.40542436	-0.24229450
H	1.04048528	-2.46335772	2.48550491
H	0.49023122	-0.79607580	2.58993403
N	-0.88339429	1.54670824	0.52890136
C	0.38188425	1.92810290	1.15024622
H	0.16004397	2.68714193	1.89667847
H	0.85348695	1.09683697	1.65594743

H	1.06511392	2.35291283	0.41387321
F	-2.95755417	-2.03008977	-1.29217553
H	-2.70638883	-1.14647122	-0.92448703

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Ac-Pro-NMe2-endo-alpha-HFdonor-HFHFacceptor

optimized M062X/junccpVTZ/H2O

0 1

N	1.26957927	0.92463363	0.05027366
O	1.66885161	-1.10249960	0.88418800
O	-2.08065328	-0.38035496	0.53290645
C	1.62469333	2.19230205	-0.60785066
C	0.26595480	2.83788076	-0.87111378
C	-0.60479670	2.32702568	0.27685563
C	-0.11323424	0.88599527	0.49521648
C	2.10324359	-0.07876478	0.32265700
C	3.53430135	0.06877661	-0.09426288
C	-1.03145117	-0.15563078	-0.13495811
C	-1.69547484	-1.91005223	-1.61760685
H	-0.13740080	0.62158242	1.55214457
H	2.19096674	2.00622094	-1.51910525
H	2.23344440	2.79909387	0.06310545
H	-1.67062422	2.37066262	0.06906828
H	-0.41088276	2.89594934	1.18440582
H	4.11317088	-0.76439159	0.29078445
H	3.94492294	1.00915383	0.27052323
H	3.59728896	0.07796690	-1.18359603
H	-1.14955669	-2.58354075	-2.27102061
H	-2.57358891	-1.52973413	-2.13839452
H	-2.00713835	-2.44716332	-0.72727612
H	0.33375185	3.92158984	-0.89468546
H	-0.13559043	2.50639076	-1.82876983
N	-0.79750632	-0.81067525	-1.25217585
C	0.26993418	-0.54541403	-2.21695539

H	-0.12778264	-0.75947404	-3.20547136
H	0.57771946	0.49058230	-2.20184128
H	1.12348353	-1.19781356	-2.03110737
F	-4.35459391	-1.26563059	-0.05995919
H	-3.46621115	-0.95171277	0.11990860
F	-2.49520098	0.94040809	2.59826608
H	-2.33684888	0.41690818	1.80000166
F	3.20341521	-2.93629022	1.37713308
H	2.58917425	-2.19623987	1.17703718

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34 35 1.0
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Ac-Pro-NMe2-endo-alpha-HFdonor

optimized M062X/junccpVTZ/H2O

0 1

N	-0.28656586	1.08585270	-0.12228176
O	-1.72939815	-0.51710248	-0.68940603
O	1.90250515	-1.43939070	-1.52184001
C	0.12187514	2.33224841	0.54245495
C	1.63506178	2.35874610	0.33672238
C	1.83022816	1.62045283	-0.98789149
C	0.76045474	0.51824050	-0.96435915
C	-1.49817958	0.54263617	-0.07169237
C	-2.53938841	1.22735208	0.76188448
C	1.32864547	-0.86050072	-0.60012456
C	1.64951041	-2.78434245	0.81419729
H	0.35378024	0.34720344	-1.95909111
H	-0.16657006	2.32195618	1.59255591
H	-0.35979207	3.18299378	0.05867878
H	2.82918730	1.21248062	-1.11521043
H	1.62493852	2.29013434	-1.82167203

H	-3.50087249	0.74705266	0.61202761
H	-2.60626807	2.28323387	0.50379762
H	-2.26440126	1.16064664	1.81583124
H	2.58759749	-2.81262327	1.37074085
H	1.78797307	-3.25970498	-0.14919387
H	0.88931021	-3.31910116	1.38266036
H	2.01829119	3.37491935	0.31146036
H	2.14097550	1.83084568	1.14455788
N	1.21046682	-1.40736028	0.62343902
C	0.67417694	-0.78260917	1.82543462
H	1.16437826	-1.24322029	2.68063693
H	0.88608067	0.27815626	1.86541517
H	-0.40129567	-0.94837768	1.91795478
F	-3.95098994	-1.49817712	-0.59360561
H	-3.05087403	-1.09384535	-0.62658875

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Ac-Pro-NMe2-endo-alpha-HFHFacceptor

optimized M062X/junccpVTZ/H2O

0 1

N	-1.64020942	0.35784364	-0.11519242
O	-1.38645047	-0.83890770	-1.99384609
O	1.96596546	0.21017443	-0.43388588
C	-2.40055777	0.91360623	1.01057389
C	-1.31544252	1.53001112	1.89275760
C	-0.23397399	1.94627577	0.89530671
C	-0.27678332	0.83983345	-0.17259621
C	-2.12119202	-0.43733787	-1.09548443
C	-3.57389684	-0.81415848	-0.99886895
C	0.84099595	-0.18370965	-0.00935546
C	1.84584304	-2.31089613	0.41163437
H	-0.08159478	1.24917188	-1.16435650
H	-2.96519011	0.13318572	1.51982556
H	-3.10215942	1.67044321	0.65581955

H	0.75210406	2.05553549	1.33972840
H	-0.49886081	2.88949936	0.42055848
H	-3.85156475	-1.37895617	-1.88229939
H	-4.20075487	0.07274827	-0.91130052
H	-3.74144771	-1.42540270	-0.11060523
H	1.46384636	-3.32455723	0.48007057
H	2.54782562	-2.13150909	1.22516326
H	2.35507473	-2.18197116	-0.53863041
H	-1.69240409	2.36683569	2.47403061
H	-0.92288480	0.78963318	2.59010854
N	0.70828069	-1.39128591	0.49772370
C	-0.47633022	-1.93063637	1.16691034
H	-0.12925065	-2.62532611	1.92693063
H	-1.04614144	-1.15514599	1.65910693
H	-1.10574223	-2.46803579	0.45720144
F	4.33415265	-0.40323716	0.10373179
H	3.40907419	-0.22164981	-0.08081210
F	2.20546784	2.51639636	-1.31924983
H	2.10889353	1.61310215	-0.98200785

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Ac-Pro-NMe2-endo-alpha-HFHFdonor-HFHFacceptor

optimized M062X/junccpVTZ/H2O

0 1

N	-1.20851594	1.08461556	-0.09366799
O	-1.90593960	-1.00323034	-0.54437739
O	2.16971639	-0.27833192	-0.36903717
C	-1.42630454	2.48095873	0.33892614
C	-0.01749503	3.06311123	0.35256187
C	0.68816495	2.29301324	-0.76128888
C	0.14570724	0.86567245	-0.59136530
C	-2.15784860	0.16456661	-0.15312663

C	-3.53483718	0.54350996	0.28885000
C	1.09344306	-0.00700841	0.22873506
C	1.73694441	-1.53564557	1.94672110
H	0.09455387	0.34526337	-1.54926337
H	-1.91554251	2.50902458	1.31084641
H	-2.06053281	2.98848622	-0.38783698
H	1.77202436	2.32684900	-0.70245843
H	0.38148861	2.66655047	-1.73683599
H	-4.22453425	-0.26614637	0.07595110
H	-3.86133182	1.45348646	-0.21158882
H	-3.52763576	0.73765228	1.36263525
H	1.17164301	-2.13904890	2.65088626
H	2.58969302	-1.08609182	2.45417488
H	2.08349125	-2.16175908	1.13058138
H	-0.02484591	4.13610889	0.18625749
H	0.46616934	2.87202921	1.31160266
N	0.84126243	-0.50075487	1.42299388
C	-0.21739303	-0.07681609	2.34127505
H	0.17215201	-0.18574590	3.34969851
H	-0.47359296	0.96479556	2.20049282
H	-1.10010922	-0.70781977	2.23695139
F	4.45461662	-0.86810045	0.49075074
H	3.56325304	-0.66026042	0.20434451
F	2.37363367	0.27067732	-2.78464976
H	2.31129375	0.05130755	-1.84473145
F	-3.75673969	-2.67813463	-0.64482652
H	-3.04444612	-2.03011660	-0.60634977
F	0.13457370	-2.34540323	-1.11438355
H	-0.62967709	-1.80861564	-0.90307119

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Ac-Pro-NMe2-endo-alpha-HFHFdonor

optimized M062X/junccpVTZ/H2O

0 1

N	-0.10069221	1.23477364	-0.17007580
O	-1.78834967	-0.22810523	-0.42393661
O	2.13797716	-1.52280354	-1.03505782
C	0.46340766	2.52221137	0.28249699
C	1.95452087	2.36304932	0.00750300
C	1.98277159	1.44948536	-1.21593350
C	0.87296342	0.43523152	-0.91788418
C	-1.36193962	0.88224615	-0.00946463
C	-2.27565305	1.82360813	0.71009439
C	1.43125167	-0.85317287	-0.28807269
C	1.51361862	-2.61326264	1.33333822
H	0.40491337	0.07509640	-1.83377311
H	0.23176495	2.69470147	1.33197890
H	0.03411873	3.33191849	-0.30824259
H	2.93709254	0.95873604	-1.37909837
H	1.72094948	2.01258484	-2.11083372
H	-3.29871826	1.47090562	0.63375911
H	-2.19566982	2.82872435	0.30054198
H	-1.98938862	1.86864428	1.76245214
H	0.79489378	-2.99087342	2.05745775
H	2.50849656	-2.62068095	1.78284898
H	1.51603117	-3.24987167	0.45533542
H	2.43606686	3.32169610	-0.16175206
H	2.44738514	1.87871751	0.85173758
N	1.11900741	-1.26103873	0.95550436
C	0.59522708	-0.44677534	2.04636481
H	1.02389023	-0.82344012	2.97266199
H	0.89437720	0.59073322	1.95629585
H	-0.49137934	-0.51829211	2.12087500
F	-4.17347108	-0.83177911	-0.07786289
H	-3.24567571	-0.59075754	-0.20900813
F	-0.88662927	-2.27427491	-1.54745477
H	-1.17048090	-1.46865641	-1.11207670

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Ac-Pro-NMe2-endo-alpha-HFtrans

optimized M062X/junccpVTZ/H2O

0 1

N	-1.52060990	0.22010090	-0.29537756
O	-1.14657500	-1.67570619	-1.43527252
O	2.02260158	0.38916375	-0.96336147
C	-2.31879510	1.12667200	0.53830640
C	-1.32107894	2.21738514	0.92535431
C	-0.35750647	2.26217326	-0.26121558
C	-0.25912327	0.79695041	-0.71835079
C	-1.89600293	-0.99913313	-0.73469198
C	-3.25254401	-1.48121560	-0.29641211
C	1.02825119	0.11390243	-0.25908620
C	2.37431128	-1.43423189	0.97329820
H	-0.17680695	0.73452297	-1.80274508
H	-2.72609749	0.60214316	1.40226774
H	-3.15038550	1.53653917	-0.03785978
H	0.61485280	2.68209274	-0.01728151
H	-0.78792321	2.84912212	-1.07115205
H	-3.47763256	-2.41196497	-0.80615710
H	-4.02186860	-0.74120921	-0.51404380
H	-3.25469219	-1.65090140	0.78162871
H	2.16240404	-2.33811809	1.53703013
H	3.08878403	-0.82311297	1.52492815
H	2.80559492	-1.70337649	0.01359756
H	-1.81228723	3.17045300	1.10129500
H	-0.78879842	1.94444335	1.83637686
N	1.11621446	-0.71639548	0.77352337
C	0.08121277	-0.99984878	1.76377513
H	0.57710482	-1.17893023	2.71473524
H	-0.59089530	-0.16377724	1.89516228
H	-0.48493273	-1.89120458	1.48925283
F	4.43455535	0.35580170	-0.56741741
H	3.46278973	0.33154184	-0.68409166

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Ac-Pro-NMe2-endo-alpha-thioureaacceptor

optimized M062X/junccpVTZ/H2O

0 1

N	-2.58907226	-0.67635340	0.29448281
O	-2.33106357	0.57501818	2.13932624
O	0.87994737	0.32390983	0.07512999
C	-3.37395318	-1.39514970	-0.71539314
C	-2.33537368	-1.75296566	-1.77762595
C	-1.03931092	-1.89885686	-0.98014505
C	-1.15660188	-0.83138922	0.12134410
C	-3.08096114	0.01044618	1.34564510
C	-4.58011411	0.06942982	1.46560979
C	-0.33182306	0.42202322	-0.17540044
C	0.07304005	2.70087396	-0.74708025
H	-0.71561221	-1.18547900	1.05248832
H	-4.17519664	-0.76748657	-1.10446394
H	-3.82039864	-2.29115386	-0.28002404
H	-0.14188889	-1.77077727	-1.58023718
H	-0.99657859	-2.88019995	-0.50995344
H	-4.84054012	0.53627075	2.40953843
H	-5.01989027	-0.92538261	1.40665979
H	-4.99222000	0.66086185	0.64600892
H	0.69632939	2.63532919	-1.64011990
H	0.71492974	2.73231396	0.12889927
H	-0.51933679	3.60998767	-0.79081147
H	-2.60196393	-2.65952750	-2.31404322
H	-2.24246878	-0.95011501	-2.50882648
N	-0.83537403	1.55992517	-0.65845616
C	-2.19700303	1.79739067	-1.12712508
H	-2.14827241	2.53602986	-1.92352424
H	-2.64459852	0.90271169	-1.53821752
H	-2.82596489	2.18861782	-0.32548629
C	4.16670789	-0.20977404	0.21371741
N	3.28610068	-1.14125502	0.58784021
H	3.62861640	-2.01748800	0.93772936
H	2.28931321	-0.95791821	0.53513082
N	3.65729278	0.94163967	-0.23210545
H	4.28552953	1.66732363	-0.52526091
H	2.65243688	1.07693776	-0.27374122
S	5.84540207	-0.47450909	0.29993727

1 4 1.0 7 1.0 8 1.5
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Ac-Pro-NMe2-endo-alpha-ureaacceptor

optimized M062X/junccpVTZ/H2O

0 1

N	-2.26285100	-0.61418100	0.29875000
O	-2.02362000	0.73741900	2.07354800
O	1.25007900	0.23766000	0.16804100
C	-3.03740700	-1.35569300	-0.70266000
C	-1.97348700	-1.81009100	-1.70070400
C	-0.72034100	-1.96943300	-0.84008700
C	-0.83222900	-0.83502700	0.19301900
C	-2.76560300	0.15417900	1.28575200
C	-4.26492500	0.27527900	1.34325200
C	0.05721800	0.36316900	-0.14544900
C	0.60795600	2.55886800	-0.86958700
H	-0.44194700	-1.15120300	1.15944000
H	-3.79632900	-0.71879900	-1.15608100
H	-3.53714900	-2.20834300	-0.23916100
H	0.20693400	-1.92014200	-1.40527100
H	-0.74808500	-2.92222700	-0.31330300
H	-4.54011700	0.83531900	2.23056400
H	-4.73655500	-0.70683500	1.36149500
H	-4.62918000	0.79934500	0.45798400
H	1.35175700	2.31511200	-1.62904600
H	1.11796000	2.71899800	0.07790400
H	0.08804300	3.46759600	-1.15486800
H	-2.25750300	-2.73055900	-2.20356200
H	-1.81551300	-1.04874100	-2.46462900
N	-0.37168800	1.48201200	-0.73738300
C	-1.71392200	1.75771800	-1.23975200
H	-1.62295200	2.45218600	-2.07072200
H	-2.19391400	0.86337100	-1.61351700
H	-2.33841100	2.21436800	-0.46956800
C	4.58087800	-0.37060400	0.32731000
N	3.66125000	-1.26904600	0.77258500
H	3.96635400	-2.22173500	0.86174200
H	2.67508600	-1.07214100	0.66398300
N	4.08509300	0.86548000	0.04391100
H	4.70469900	1.50119500	-0.42618100
H	3.08549100	0.98812900	-0.05425400
O	5.77977500	-0.63944700	0.23784300

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Ac-Pro-NMe2-endo-PPII-2H2Oacceptor3H2O

5 H2O optimized M062X/junccpVTZ/H2O

0 1

N	-1.21828300	-1.54003200	-0.00507400
O	0.19052200	-1.36945000	-1.73521100
O	-0.07396500	0.83577200	0.65398100
C	-1.75498000	-2.14715900	1.21721300
C	-2.59412500	-1.01913800	1.80990200
C	-3.10535400	-0.27430800	0.57510900
C	-1.90182300	-0.31519800	-0.38477900
C	-0.21565300	-2.01246300	-0.76069300
C	0.36872000	-3.33913300	-0.36569100
C	-0.99100000	0.89282600	-0.18268100
C	-0.31922200	3.12889500	-0.75114400
H	-2.19519100	-0.38091300	-1.42920000
H	-0.94773500	-2.46414500	1.87476600
H	-2.36852800	-3.01619300	0.97052000
H	-3.43105200	0.74082300	0.79244600
H	-3.93662900	-0.81189900	0.12020600
H	1.07224300	-3.65543800	-1.12827800
H	-0.41521800	-4.08529100	-0.23965000
H	0.89337300	-3.23637200	0.58490900
H	-0.36292500	3.71644500	-1.66454000
H	0.69698800	2.77349100	-0.60092200
H	-0.61017300	3.75492200	0.09327400
H	-3.39779800	-1.39016200	2.44007000
H	-1.95886100	-0.36395900	2.40521200
N	-1.22212900	1.99281400	-0.89347800

C	-2.36040500	2.18703700	-1.78253800
H	-2.04769600	2.12008600	-2.82480300
H	-3.14319300	1.46219900	-1.59159000
H	-2.77248800	3.17836700	-1.60216400
H	1.05781700	-0.54304500	1.14359500
O	1.88190200	-0.99548400	1.39470600
H	2.53002900	-0.27384400	1.37390400
O	2.24096900	0.56528900	-1.72017400
H	1.44201100	0.02064100	-1.63017000
H	2.43919300	0.90957900	-0.83493500
O	3.21887000	1.45603100	0.83313400
H	4.10592500	1.82457700	0.85680600
H	2.64952900	2.03354200	1.38154500
O	1.21348900	2.71548100	2.17468100
H	1.11982100	2.50411500	3.10775500
H	0.61832300	2.10470100	1.69695900
O	3.47444300	-1.92220400	-0.82968800
H	2.87789300	-1.84000800	-0.06989700
H	3.24043200	-1.14333400	-1.35556600

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Ac-Pro-NMe2-endo-PPII-guanidinium

optimized M062X/junccpVTZ/H2O

1 1 0 1 1 1

N(Fragment=1)	0.50962700	1.55901600	0.25073500
O(Fragment=1)	1.51527300	1.83003500	-1.73594100
O(Fragment=1)	0.06903500	-0.97464700	-0.69306700
C(Fragment=1)	-0.42345900	1.91487500	1.32360300
C(Fragment=1)	-0.34509700	0.70071000	2.24137800
C(Fragment=1)	1.11777400	0.26965300	2.11797600
C(Fragment=1)	1.43168800	0.50127600	0.62698000
C(Fragment=1)	0.66865900	2.19964500	-0.92543100
C(Fragment=1)	-0.23632800	3.37650300	-1.17879800
C(Fragment=1)	1.18188300	-0.76577400	-0.18853600
C(Fragment=1)	2.04087400	-2.85306500	-1.06964200
H(Fragment=1)	2.45191700	0.83982400	0.46274900
H(Fragment=1)	-1.42472200	2.08262900	0.93248300
H(Fragment=1)	-0.09094600	2.82180900	1.83448300
H(Fragment=1)	1.28671000	-0.76057000	2.42471600
H(Fragment=1)	1.75572900	0.91547700	2.72035600
H(Fragment=1)	0.03676700	3.83309100	-2.12411700
H(Fragment=1)	-0.14702000	4.10742500	-0.37511600
H(Fragment=1)	-1.27880200	3.06084900	-1.21852000
H(Fragment=1)	2.87090900	-2.92564900	-1.77151400
H(Fragment=1)	1.10481400	-2.82140500	-1.61414900
H(Fragment=1)	2.05541000	-3.72522200	-0.41588000
H(Fragment=1)	-0.63248200	0.93302400	3.26324500
H(Fragment=1)	-1.00204800	-0.08504900	1.86489400
N(Fragment=1)	2.18764200	-1.63616500	-0.28399600
C(Fragment=1)	3.49558300	-1.43032300	0.32992100
H(Fragment=1)	4.13961400	-0.82295100	-0.30730700
H(Fragment=1)	3.40798200	-0.96463700	1.30709000
H(Fragment=1)	3.95816600	-2.40435100	0.46678800
C(Fragment=2)	-3.14594300	-1.02502400	-0.22438600
N(Fragment=2)	-2.53182400	0.04279700	-0.71816400
H(Fragment=2)	-3.06488100	0.81032500	-1.08837700
H(Fragment=2)	-1.51934900	0.00816700	-0.83097100
N(Fragment=2)	-2.42125000	-2.07798800	0.13211800
H(Fragment=2)	-2.85341400	-2.89705400	0.52250000
H(Fragment=2)	-1.42455700	-2.06771000	-0.05183800
N(Fragment=1)	-4.46682500	-1.03605300	-0.07626800
H(Fragment=1)	-4.94040800	-1.84594400	0.28419300
H(Fragment=1)	-5.01926200	-0.22728200	-0.30300800

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Ac-Pro-NMe2-endo-PPII-H2OcisHFtrans

M062X/junccpVTZ/H2O optimized

0 1

N	1.39959570	-0.64035340	-0.12436034
O	1.04231610	-0.21841143	-2.29855841
O	-0.75890537	0.98111179	0.11760890
C	2.19473275	-0.66607102	1.10801383
C	1.14047297	-0.95110377	2.17131553
C	0.15313407	-1.86394229	1.44272938
C	0.09543663	-1.25788091	0.02676307
C	1.79774290	-0.18279860	-1.32906767
C	3.19398142	0.37272283	-1.40479193
C	-1.01990693	-0.22295963	-0.08526949
C	-3.30734530	0.36457878	-0.50399329
H	-0.04169930	-2.00860883	-0.74772040
H	2.69852304	0.28552083	1.25743991
H	2.93890675	-1.46496913	1.06261825
H	-0.82382769	-1.90906330	1.91929239
H	0.54976040	-2.87642427	1.37463503
H	3.42675013	0.60175361	-2.43955992
H	3.91798585	-0.33962679	-1.01016742
H	3.25163119	1.28084786	-0.80377443
H	-4.15843004	-0.10867159	-0.98394464
H	-2.96339912	1.19151380	-1.12016817
H	-3.61010560	0.74889907	0.47012152
H	1.56116692	-1.40964972	3.06210403
H	0.65023829	-0.01937085	2.45672084
N	-2.24904163	-0.63128688	-0.36331467
C	-2.65564072	-2.02546446	-0.49879913
H	-2.87551737	-2.25351932	-1.54139386
H	-1.89202810	-2.70119729	-0.13377422
H	-3.55489411	-2.18148829	0.09446204
H	0.84173375	1.85135590	0.48904484
O	1.57679368	2.44501621	0.71585007
H	1.16117773	3.28917441	0.91107887
F	-1.99853062	3.07159277	0.54432806
H	-1.58235756	2.21645271	0.35715147

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Ac-Pro-NMe2-endo-PPII-H2Ocis

M062X/junccpVTZ/H2O optimized

0 1

N	-1.11427300	0.36524160	-0.54173225
O	-0.80693131	-1.54685668	-1.67682660
O	0.62938326	-0.86001751	1.17177848
C	-1.91565124	1.36861662	0.16577951
C	-0.85382397	2.18106059	0.89739849
C	0.33391017	2.14708951	-0.06600616
C	0.29352299	0.71037768	-0.61981397
C	-1.57203947	-0.76496552	-1.11273039
C	-3.05351974	-1.01178913	-1.01233779
C	1.13913541	-0.23286262	0.23981213
C	3.29493502	-1.21842821	0.72195680
H	0.62266740	0.64723040	-1.65411169
H	-2.61681749	0.88839162	0.84335983
H	-2.46731730	1.98590671	-0.54773730
H	1.28146950	2.38064797	0.41497767
H	0.18094453	2.85043244	-0.88431620
H	-3.30927139	-1.87863665	-1.61289272
H	-3.61847224	-0.14439578	-1.35275394
H	-3.31290967	-1.19545388	0.03085835
H	4.00999364	-1.68021032	0.04279834
H	2.68609753	-1.98488767	1.18770005
H	3.84406854	-0.67468549	1.49266393
H	-1.18485940	3.19076079	1.12563534
H	-0.59323821	1.67820001	1.82929699
N	2.44722806	-0.31450545	-0.04012973
C	3.14060534	0.47703333	-1.04544474
H	3.37248844	-0.12948246	-1.92214168
H	2.56209336	1.34154304	-1.34974562
H	4.07486191	0.83768124	-0.61626309
H	-1.04818685	-0.96365040	1.76588121
O	-1.93201150	-1.07612376	2.16705427
H	-1.78026839	-1.57735460	2.97209201

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Ac-Pro-NMe2-endo-PPII-HFcis

M062X/junccpVTZ/H2O optimized

0 1

N	-1.15920472	0.31227338	-0.53183760
O	-0.82066168	-1.69262763	-1.47974551
O	0.66073821	-0.75933105	1.23163492
C	-1.96404676	1.34954317	0.12065055
C	-0.90277184	2.23029578	0.76905113
C	0.26353270	2.14942064	-0.21704020
C	0.23845409	0.67654162	-0.66819186
C	-1.59678739	-0.88331568	-0.97417544
C	-3.06431709	-1.16483111	-0.79979849
C	1.12294105	-0.18863980	0.22679002
C	3.26952669	-1.13391178	0.75336475
H	0.54860239	0.54600396	-1.70217502
H	-2.64241702	0.90675538	0.84475875
H	-2.54183742	1.90434382	-0.62246080
H	1.21689844	2.43624585	0.22155907
H	0.07673644	2.78636466	-1.08125990
H	-3.30847163	-2.09350137	-1.30492470
H	-3.66983792	-0.35270759	-1.20077516
H	-3.28479516	-1.25536830	0.26431880
H	4.11980899	-1.44842488	0.15387069
H	2.71500721	-2.00528670	1.08592091
H	3.62885752	-0.58477680	1.62446153
H	-1.24833091	3.24764169	0.93171673
H	-0.61240907	1.80188014	1.72915885
N	2.41432106	-0.28896357	-0.07250036
C	3.08186978	0.43782016	-1.14535977
H	3.29169427	-0.22613206	-1.98413696
H	2.49026326	1.27852949	-1.48807871
H	4.02298041	0.82734526	-0.76124936
F	-1.58764993	-0.92593827	2.15448737
H	-0.71073446	-0.82050539	1.72241527

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Ac-Pro-NMe2-endo-PPII-HFdonor-HFHFacceptor

M062X/junccpVTZ/H2O optimized

0 1

N	-1.12161259	0.87232532	-0.43853712
O	-1.50187327	-1.29664864	-0.76978304
O	0.94695221	-0.22301709	0.97422935
C	-1.43483595	2.22664799	0.03738236
C	-0.06329005	2.88954697	0.05594695
C	0.65129230	2.24713851	-1.13422311
C	0.18155106	0.77988715	-1.07966288
C	-1.91013084	-0.19613500	-0.34796800
C	-3.25966708	-0.02109952	0.27738233
C	1.13542669	-0.08020770	-0.26101942
C	3.05068102	-1.51839400	-0.10183524
H	0.06465278	0.33634479	-2.06478846
H	-1.90081267	2.18350119	1.01789120
H	-2.10954908	2.71938560	-0.66491020
H	1.73389691	2.33945205	-1.08524602
H	0.30923532	2.68776317	-2.06965099
H	-3.83367991	-0.93523770	0.16505616
H	-3.78957878	0.81158906	-0.18278849
H	-3.13059043	0.20258372	1.33671226
H	3.60619871	-2.12917840	-0.80645637
H	2.46332068	-2.16281818	0.54654979
H	3.74668683	-0.93676474	0.50175576
H	-0.12574036	3.97089114	-0.02633762
H	0.45160201	2.63946917	0.98403369
N	2.16628211	-0.63744047	-0.86266641
C	2.51632766	-0.42709971	-2.26563064
H	2.20384533	-1.28195722	-2.86436600
H	2.06928037	0.47924850	-2.65661059
H	3.59662961	-0.32250504	-2.33070911
F	2.43917433	-0.81851253	2.91007072

H	1.91960508	-0.61909998	2.13022339
F	-0.90221028	0.43647886	2.50767393
H	-0.22688975	0.21269968	1.85690622
F	-2.95416508	-3.24376962	-0.60956403
H	-2.37075027	-2.45171350	-0.67027006

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34 35 1.0
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Ac-Pro-NMe2-endo-PPII-HFdonor

M062X/junccpVTZ/H2O optimized

0 1

N	-0.83543153	0.93848584	-0.18021140
O	-1.63522457	-1.12806655	-0.44669720
O	0.77049642	-0.29819062	1.58076374
C	-0.89580746	2.33987933	0.25632162
C	0.57017558	2.76567329	0.25367017
C	1.19431239	1.89351800	-0.83669704
C	0.48573950	0.54377618	-0.64533210
C	-1.82247635	0.05714011	-0.09671055
C	-3.14438117	0.53124237	0.43007187
C	1.18308161	-0.30790121	0.42599329
C	2.97665579	-1.83552318	0.99910603
H	0.38228717	-0.02197036	-1.56691964
H	-1.35439794	2.41672560	1.23976207
H	-1.48473347	2.92311922	-0.45353499
H	2.27517160	1.81175791	-0.74764847
H	0.95665109	2.28470469	-1.82562959
H	-3.89825147	-0.23150140	0.26335038
H	-3.44316621	1.46197762	-0.04891413
H	-3.05774723	0.71971739	1.50100785
H	3.10662187	-2.83686883	0.58776718

H	2.41016120	-1.88913610	1.92119284
H	3.96232559	-1.41187975	1.19956312
H	0.68601384	3.82869362	0.06165983
H	1.02191790	2.53577496	1.21770149
N	2.26296788	-1.01227587	0.03743410
C	2.83614622	-1.01779199	-1.29801282
H	2.70993551	-1.99853777	-1.75943197
H	2.38823104	-0.26731007	-1.93775830
H	3.90345609	-0.80508109	-1.22606931
F	-3.46844291	-2.70678042	-0.33910298
H	-2.72409637	-2.05265168	-0.37772570

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Ac-Pro-NMe2-endo-PPII-HFHFacceptor

M062X/junccpVTZ/H2O optimized

0 1

N	1.46559277	-0.54772344	-0.10225789
O	1.04822545	-0.12827675	-2.26401511
O	-0.79916253	0.97236468	0.12818550
C	2.26302289	-0.51293748	1.12794318
C	1.22211612	-0.81541083	2.19977169
C	0.27298163	-1.78611697	1.49597942
C	0.19380359	-1.22395228	0.06238606
C	1.81996123	-0.06072310	-1.30971021
C	3.18271093	0.56805842	-1.40430759
C	-0.97153241	-0.25499893	-0.08669505
C	-3.26777734	0.20001615	-0.62158227
H	0.09337485	-2.00241367	-0.68999875
H	2.72777397	0.46150178	1.25355956
H	3.03934361	-1.28113826	1.09893551
H	-0.70226332	-1.85665203	1.97274263
H	0.70906183	-2.78349396	1.45470286
H	3.39433319	0.79900244	-2.44308232
H	3.94763270	-0.09859462	-1.00760628

H	3.19690755	1.48493567	-0.81442642
H	-4.04085162	-0.31747926	-1.18092124
H	-2.92812015	1.06059976	-1.19167469
H	-3.67542899	0.53855227	0.33053286
H	1.66102746	-1.23502243	3.10080936
H	0.69394877	0.10150160	2.46453236
N	-2.15902255	-0.72809303	-0.40954260
C	-2.46544181	-2.14902161	-0.55826219
H	-2.48710278	-2.42419153	-1.61235904
H	-1.74734881	-2.76705776	-0.03248566
H	-3.44527072	-2.32903879	-0.12269844
F	-2.30755321	2.88730671	0.71618723
H	-1.78878442	2.11797406	0.47043317
F	1.22040747	2.35441283	0.59325817
H	0.49851487	1.74407048	0.40009795

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Ac-Pro-NMe2-endo-PPII-HFHFdonor-HFHFacceptor

M062X/junccpVTZ/H2O optimized

0 1

N	-1.03903123	1.07183094	-0.36248591
O	-1.55331060	-1.06654826	-0.82361172
O	0.79804848	-0.20065375	1.15959850
C	-1.35423201	2.42744159	0.12826686
C	0.01911934	3.07830397	0.20928081
C	0.77426920	2.43868577	-0.95487661
C	0.31641523	0.96964896	-0.89481523
C	-1.89312434	0.06337991	-0.38370350
C	-3.27414757	0.29629351	0.13917856
C	1.21162810	0.13716991	0.02199467
C	3.27359335	-0.98568698	0.48340779
H	0.28139854	0.49793592	-1.87456655

H	-1.86033421	2.36973178	1.08730481
H	-1.99501461	2.93322536	-0.59506932
H	1.85322912	2.54034339	-0.87489732
H	0.45259880	2.86756751	-1.90290802
H	-3.89654574	-0.56691807	-0.07171594
H	-3.70797361	1.18721746	-0.31175600
H	-3.21797209	0.45497398	1.21667093
H	4.28667595	-0.94746214	0.09639728
H	2.92974350	-2.02034505	0.49829067
H	3.25766750	-0.58547317	1.49328101
H	-0.03536454	4.16015222	0.13236516
H	0.49556325	2.82120041	1.15636765
N	2.42063003	-0.18162677	-0.38870291
C	2.91776172	0.02072893	-1.74503188
H	2.97972264	-0.94409232	-2.24746193
H	2.27454805	0.67708291	-2.31684946
H	3.90822690	0.46724021	-1.69060185
F	1.37464442	-2.04021464	2.79055479
H	1.21699179	-1.35866030	2.13940640
F	-1.09344647	0.58734800	2.58256417
H	-0.38842255	0.32070955	1.98364012
F	-3.23143515	-2.90510655	-0.87577954
H	-2.58352084	-2.18884839	-0.85056561
F	0.55263374	-2.06323719	-1.73448412
H	-0.24957945	-1.66429428	-1.38481098

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Ac-Pro-NMe2-endo-PPII-HFHFdonor

M062X/junccpVTZ/H2O optimized

0 1

N	-0.80745135	1.11761616	-0.19056901
O	-1.74610016	-0.92328740	-0.28549572
O	0.70427527	-0.10681750	1.63436610
C	-0.81692910	2.55533116	0.13403472
C	0.65848102	2.93529508	0.07065919
C	1.22853522	1.96663511	-0.96493102
C	0.50451908	0.65336884	-0.63243330
C	-1.83494839	0.31074224	-0.03376127
C	-3.12663750	0.88768846	0.45461342
C	1.19868948	-0.10452464	0.51270421
C	3.01897413	-1.47529661	1.27164763
H	0.38457741	0.00186737	-1.49497236
H	-1.25693032	2.72059369	1.11442201
H	-1.40163000	3.09147217	-0.61434977
H	2.30919010	1.86964705	-0.90526932
H	0.96003752	2.27868297	-1.97379357
H	-3.92165462	0.15937717	0.33302515
H	-3.37283744	1.80132425	-0.08249108
H	-3.02833167	1.13611670	1.51237660
H	4.08803301	-1.50532174	1.07361251
H	2.63194147	-2.49732771	1.28549025
H	2.83926358	-1.01564682	2.23744587
H	0.79804387	3.97727079	-0.20226212
H	1.12705093	2.76458434	1.03950866
N	2.37226260	-0.69653638	0.22799179
C	2.87205893	-0.93493353	-1.11629295
H	2.64912353	-1.95782454	-1.42538624
H	2.43821367	-0.25007058	-1.83540620
H	3.95125626	-0.78929980	-1.12203198
F	-3.73592790	-2.37145126	-0.01472915
H	-2.96072479	-1.79717057	-0.11759520
F	0.12532795	-2.47481428	-0.81287264
H	-0.57475970	-1.84444089	-0.60427325

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Ac-Pro-NMe2-endo-PPII-HFtrans

M062X/junccpVTZ/H2O optimized

0 1

N	1.58401009	-0.22363546	-0.10706789
O	1.28578520	0.94406492	-2.00075020
O	-0.73544342	0.97177311	0.53262272
C	2.25204158	-0.54142891	1.15911429
C	1.21135853	-1.38099192	1.89634615
C	0.44794822	-2.07201452	0.76557516
C	0.36432702	-0.97818420	-0.31248671
C	1.95825683	0.71491835	-0.99662566
C	3.22846257	1.46285770	-0.68950660
C	-0.86177987	-0.08876256	-0.10416586
C	-3.20063222	0.36270709	-0.40440678
H	0.35122574	-1.37651069	-1.32362696
H	2.51374310	0.36608673	1.69954196
H	3.16460766	-1.11128293	0.97147165
H	-0.52986335	-2.43717094	1.07191034
H	1.02118644	-2.91069513	0.37143322
H	3.51509658	2.04223319	-1.56096319
H	4.03312579	0.78340030	-0.41216668
H	3.06039619	2.13879331	0.15012773
H	-3.98606273	0.01328260	-1.06805735
H	-2.95366419	1.39204023	-0.65197745
H	-3.55545175	0.32322949	0.62574133
H	1.66472260	-2.08395278	2.58991214
H	0.54038464	-0.72838808	2.45403206
N	-2.03299290	-0.49234211	-0.58691400
C	-2.27915441	-1.77718226	-1.22900985
H	-2.57285321	-1.62330099	-2.26694439
H	-1.40488627	-2.41526689	-1.19744586
H	-3.08893645	-2.28410125	-0.70532726
F	-2.23032847	2.60614549	1.57920481
H	-1.68463858	1.92992065	1.13338368

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Ac-Pro-NMe2-endo-PPII-thioureaacceptor

M062X/junccpVTZ/H2O optimized

0 1 0 1 0 1

N(Fragment=1)	0.84231840	1.53280005	0.29123309
O(Fragment=1)	1.96695008	1.79730744	-1.63218055
O(Fragment=1)	0.34849704	-0.95735327	-0.74547454
C(Fragment=1)	-0.15143472	1.89505325	1.30506494
C(Fragment=1)	-0.19149013	0.65097719	2.18417291
C(Fragment=1)	1.25601074	0.15630626	2.14950202
C(Fragment=1)	1.68848370	0.42259874	0.69392709
C(Fragment=1)	1.08516137	2.17983905	-0.86544599
C(Fragment=1)	0.22155584	3.37888108	-1.15832084
C(Fragment=1)	1.44037499	-0.80357962	-0.18474020
C(Fragment=1)	2.28467034	-2.87552664	-1.11765073
H(Fragment=1)	2.73097672	0.72061899	0.61647357
H(Fragment=1)	-1.11314331	2.11652615	0.84755787
H(Fragment=1)	0.17979270	2.77048987	1.86912273
H(Fragment=1)	1.35748819	-0.89079282	2.42761819
H(Fragment=1)	1.87695136	0.75121585	2.81848567
H(Fragment=1)	0.58194130	3.86020559	-2.06123875
H(Fragment=1)	0.24231655	4.08366753	-0.32749096
H(Fragment=1)	-0.81507661	3.07348092	-1.30377660
H(Fragment=1)	3.12372696	-2.91915460	-1.81177663
H(Fragment=1)	1.35595369	-2.81010158	-1.67164568
H(Fragment=1)	2.28541412	-3.77972736	-0.50876670
H(Fragment=1)	-0.53997799	0.86529405	3.19100564
H(Fragment=1)	-0.85368701	-0.09128798	1.73651958
N(Fragment=1)	2.42645775	-1.70146329	-0.26921170
C(Fragment=1)	3.71426054	-1.55513213	0.40020661
H(Fragment=1)	4.39706270	-0.93907324	-0.18688429
H(Fragment=1)	3.60209236	-1.12808141	1.39259128
H(Fragment=1)	4.14838202	-2.54534595	0.51257657
C(Fragment=2)	-2.96969244	-0.75940367	-0.27186255
N(Fragment=2)	-2.24960976	0.22501277	-0.81698754
H(Fragment=2)	-2.72797062	1.04828042	-1.13538054
H(Fragment=2)	-1.24281987	0.12386535	-0.92487194
N(Fragment=2)	-2.29191584	-1.85173000	0.09386026
H(Fragment=2)	-2.79166799	-2.62114263	0.50120803
H(Fragment=2)	-1.29641726	-1.92008766	-0.08092226
S(Fragment=2)	-4.64894189	-0.62880629	-0.04878390

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Ac-Pro-NMe2-endo-PPII-ureaacceptor

optimized M062X/junccpVTZ/H2O

0 1

N	0.04542629	1.31327922	0.42911114
O	0.24196240	0.02761593	2.25634383
O	-0.50713694	-1.11936114	-0.68551882
C	0.51789659	2.27376261	-0.57148560
C	-0.53996723	2.16023115	-1.66310330
C	-1.82108261	1.87721305	-0.87680697
C	-1.34457476	0.93485083	0.24480962
C	0.74405417	0.83675851	1.47544748
C	2.15213560	1.34644859	1.63259635
C	-1.46520319	-0.53290467	-0.17397439
C	-2.84720608	-2.52087116	-0.32234599
H	-1.88386577	1.08679818	1.17700425
H	1.51345165	2.00816219	-0.91956045
H	0.54671742	3.28102163	-0.14874104
H	-2.60659821	1.43461689	-1.48550719
H	-2.20498831	2.79533835	-0.43298079
H	2.58944714	0.90387449	2.52163384
H	2.15654377	2.43331375	1.71985386
H	2.75164786	1.08323183	0.76057525
H	-3.17243892	-3.06006856	0.56802612
H	-1.91270819	-2.93692533	-0.67901911
H	-3.61217905	-2.62419709	-1.09207571
H	-0.60555841	3.05766611	-2.27239688
H	-0.30621099	1.31603704	-2.31288288
N	-2.65835198	-1.11579159	0.00408627
C	-3.80663391	-0.45702871	0.61271084
H	-3.80597812	-0.58553337	1.69649806
H	-3.83506194	0.60131835	0.37443076
H	-4.70900536	-0.91144393	0.20972496
C	2.94767070	-1.19532932	-0.55029772
N	2.22352023	-0.55797527	-1.50347014
H	2.71167414	-0.19090423	-2.30016658
H	1.21228952	-0.60022693	-1.48750842
N	2.20727612	-1.82863451	0.40465479
H	2.69341847	-2.07415685	1.24993195
H	1.21867932	-1.62745764	0.47233382
O	4.17931126	-1.20892919	-0.54646880

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9 17 1.0 18 1.0 19 1.0
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30 31 1.0 34 1.0 37 2.0
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Ac-Pro-NMe2-exo-alpha-guanidinium

optimized M062X/junccpVTZ/H2O

1 1

N	-2.20539861	-0.54897450	0.32433986
O	-1.02428026	0.17388999	2.08738518
O	1.20074519	0.08134759	-0.44521944
C	-3.42490805	-0.97071016	-0.36992345
C	-2.88566128	-1.83374505	-1.50818008
C	-1.54764699	-1.17568156	-1.84822802
C	-1.00302518	-0.77653342	-0.46888602
C	-2.11649997	-0.09341181	1.58946343
C	-3.41188073	0.07903466	2.33697064
C	-0.00436699	0.37253116	-0.51221741
C	0.65548390	2.65688002	-0.58801340
H	-3.56562454	-1.87308329	-2.35468611
H	-0.43538206	-1.60110470	-0.03426834
H	-3.97111923	-0.10241778	-0.74988891
H	-4.08158223	-1.52030512	0.29997631
H	-1.70330130	-0.29240734	-2.46861368
H	-0.85979893	-1.83572732	-2.36921690
H	-3.21087715	0.58344537	3.27608878
H	-3.85962254	-0.89449731	2.53921962
H	-4.12614043	0.65644558	1.75022671
H	1.37160744	2.53463734	-1.39989926
H	1.18507860	2.58320864	0.36189366
H	0.19451117	3.63615820	-0.66297974
H	-2.71874994	-2.84896685	-1.14870717
N	-0.38896260	1.63994652	-0.66449490
C	-1.76553442	2.10280440	-0.77730227
H	-1.77457254	2.99390510	-1.39947456
H	-2.39373635	1.36010470	-1.25325088

H	-2.18149103	2.35171479	0.20123733
C	4.30460885	-0.53331952	0.22939179
N	3.91859633	0.68839725	-0.11330659
H	4.58043041	1.44204678	-0.17331878
H	2.93619138	0.84642524	-0.31947039
N	3.40203687	-1.50338321	0.28565236
H	3.66337016	-2.43635744	0.55159434
H	2.43474498	-1.28336677	0.06788075
N	5.58060347	-0.78306253	0.51124453
H	6.27005871	-0.05258582	0.47813741
H	5.88274272	-1.70672967	0.76769572

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Ac-Pro-NMe2-exo-alpha-H2OcisHFtrans

optimized M062X/junccpVTZ/H2O

0 1

N	1.63060455	0.19073105	0.18824949
O	0.90669701	-1.07575055	1.88909972
O	-1.92367681	0.20834848	0.41915704
C	2.64748379	0.79023927	-0.68052318
C	1.97380211	2.07653782	-1.15285077
C	0.49363871	1.69731792	-1.22367270
C	0.31782079	0.79393469	0.00613491
C	1.83461195	-0.71110831	1.16990343
C	3.23432542	-1.24477243	1.31755363
C	-0.85369789	-0.16622247	-0.11599827

C	-1.92270580	-2.21485106	-0.72698014
H	2.36716514	2.42472086	-2.10396679
H	0.07432523	1.39804777	0.88168386
H	2.87825470	0.12715318	-1.51912135
H	3.56605807	0.97567608	-0.12966752
H	0.28409464	1.14348005	-2.13950342
H	-0.17816006	2.55034283	-1.18066271
H	3.22136000	-2.07324057	2.01779146
H	3.89348230	-0.46351854	1.69753929
H	3.62995984	-1.57545642	0.35751924
H	-1.59214438	-3.20279250	-1.03111730
H	-2.71102599	-1.87399899	-1.39762536
H	-2.31657419	-2.26511375	0.28517880
H	2.11989413	2.85942744	-0.40892090
N	-0.77400399	-1.31259356	-0.77182001
C	0.38484553	-1.77380114	-1.52843674
H	0.02211351	-2.35092533	-2.37523735
H	0.96108802	-0.94231678	-1.91414248
H	1.02449768	-2.40882052	-0.91354854
H	-2.11508780	2.02636773	0.83454351
O	-2.14255363	2.99200579	0.93082790
H	-2.43357690	3.14912634	1.83254587
F	-4.30276853	-0.43194314	0.29727653
H	-3.35149143	-0.23810849	0.31275834

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30 31 1.0
31 32 1.0
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33 34 1.0
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Ac-Pro-NMe2-exo-alpha-H2Ocis

optimized M062X/junccpVTZ/H2O

0 1

N	-1.21005033	-0.38853482	0.13400488
O	-0.72910645	0.77222468	1.99186697

O	2.30713514	0.13552665	0.45508285
C	-2.10996429	-1.03603547	-0.82439412
C	-1.23728067	-2.13864280	-1.41946033
C	0.16401434	-1.52671559	-1.40367848
C	0.18553065	-0.75404984	-0.07696415
C	-1.57122199	0.35094282	1.20091544
C	-3.04146938	0.63760449	1.35776628
C	1.20797972	0.37871784	-0.05996349
C	1.90768546	2.64527457	-0.51336919
H	-1.56239898	-2.43008085	-2.41450015
H	0.50737895	-1.41174938	0.73227237
H	-2.43299057	-0.32579856	-1.59098908
H	-2.99421908	-1.42289205	-0.32426800
H	0.29265409	-0.84481703	-2.24530777
H	0.96182744	-2.26371547	-1.44179290
H	-3.17232113	1.38010995	2.13792642
H	-3.57137343	-0.27368090	1.63729187
H	-3.47265891	0.99930381	0.42468999
H	2.39353502	2.82046780	-1.47426009
H	2.65561304	2.39392074	0.22900945
H	1.38455657	3.55330621	-0.21520954
H	-1.26590002	-3.01666863	-0.77442321
N	0.94081365	1.56172704	-0.62564390
C	-0.28043154	1.91193627	-1.33499515
H	-0.02293861	2.64318078	-2.09893403
H	-0.71833809	1.05472342	-1.83160930
H	-1.01664611	2.35682253	-0.66210166
H	2.77402268	-1.51269339	0.94453742
O	3.04282652	-2.42926750	1.15008323
H	2.82895841	-2.55414879	2.07773621

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30 31 1.0
31 32 1.0
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Ac-Pro-NMe2-exo-alpha-HFcis

optimized M062X/junccpVTZ/H2O

0 1

N	1.24194656	0.24333933	0.15232404
O	0.52576998	-0.87890837	1.95469418
O	-2.32133150	0.24346276	0.39120154
C	2.25539386	0.75757104	-0.77306090
C	1.57965930	1.99309674	-1.36332076
C	0.09926973	1.60914448	-1.39092128
C	-0.07339193	0.82469905	-0.08109603
C	1.45020033	-0.57355192	1.20401371
C	2.85150382	-1.09128149	1.38950577
C	-1.24635467	-0.14538928	-0.11288470
C	-2.28001403	-2.26551654	-0.62060259
H	1.96903601	2.24756129	-2.34521967
H	-0.30866684	1.50915847	0.73548584
H	2.48257770	0.01700509	-1.54534146
H	3.17604998	0.99365816	-0.24565286
H	-0.11504813	0.97177199	-2.24937496
H	-0.57040061	2.46402025	-1.42949661
H	2.84155729	-1.86603157	2.14894570
H	3.50711597	-0.28129316	1.71106601
H	3.24802432	-1.48930800	0.45579787
H	-2.73450720	-2.37974231	-1.60476549
H	-3.01699966	-1.89604514	0.08115227
H	-1.90803867	-3.23423791	-0.28929304
H	1.72945799	2.84350259	-0.69849288
N	-1.15819829	-1.33601749	-0.69471896
C	0.01340728	-1.85827081	-1.38595203
H	-0.33845357	-2.53955205	-2.15750542
H	0.58014702	-1.07152245	-1.86844089
H	0.66008987	-2.41040691	-0.70155236
F	-2.54276660	2.42404061	1.42592853
H	-2.43682998	1.53440051	1.00484267

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11 21 1.0 22 1.0 23 1.0 25 1.0
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25 26 1.0
26 27 1.0 28 1.0 29 1.0
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30 31 1.0
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Ac-Pro-NMe2-exo-alpha-HFdonor-HFHFacceptor

optimized M062X/junccpVTZ/H2O

0 1

N	1.47907096	-0.61700668	-0.09500384
O	0.99287548	1.45962232	-0.73199077
O	-2.01879170	-0.04854768	-0.45775528
C	2.36202245	-1.72548675	0.29378788
C	1.55724782	-2.95650400	-0.11403869
C	0.10623173	-2.52595586	0.10792140
C	0.11327302	-1.06341796	-0.36042779
C	1.84413778	0.64108744	-0.33253234
C	3.27545865	1.01777431	-0.09768892
C	-0.98967272	-0.21725727	0.25132601
C	-1.97978663	1.19369458	1.90695572
H	1.82913044	-3.83376014	0.46570348
H	-0.06325231	-1.01587787	-1.43565482
H	2.54465943	-1.70107113	1.37053506
H	3.31603878	-1.65169555	-0.22081456
H	-0.15737904	-2.59262369	1.16356625
H	-0.61168698	-3.11300211	-0.45776750
H	3.37875071	2.09679365	-0.15166743
H	3.90175458	0.55926070	-0.86377801
H	3.61634659	0.65861228	0.87227229
H	-1.61188684	1.76104003	2.75554076
H	-2.86136518	0.62662291	2.20314132
H	-2.24595164	1.87840247	1.10578127
H	1.72445794	-3.17015950	-1.16911768
N	-0.91341648	0.29588270	1.46104294
C	0.17413657	0.06759203	2.40825724
H	-0.25457491	0.04950214	3.40664488
H	0.65703179	-0.88541078	2.23581638
H	0.90941974	0.87123452	2.35117683
F	-4.39544244	0.65493388	-0.04053486
H	-3.47435449	0.40868224	-0.14069885
F	-2.18058263	-0.97370495	-2.75639026
H	-2.11098846	-0.61054600	-1.86221868
F	1.64236517	3.78396131	-1.10292141
H	1.38624535	2.84739508	-0.95551064

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Ac-Pro-NMe2-exo-alpha-HFdonor

optimized M062X/junccpVTZ/H2O

0 1

N	-0.05966335	-1.13732239	-0.05497577
O	1.68846056	0.11341167	-0.64570215
O	-1.07326887	1.89849625	-1.62839514
C	-0.71469382	-2.31035174	0.53953019
C	-2.02575868	-2.39388683	-0.23615051
C	-2.35928465	-0.93018265	-0.52532006
C	-0.98750474	-0.31736337	-0.83918554
C	1.24215158	-0.87466589	-0.02671368
C	2.13030034	-1.78746802	0.76620580
C	-0.93019595	1.19603850	-0.63011596
C	-0.62861053	3.15122525	0.75681054
H	-2.80283306	-2.90373595	0.32638529
H	-0.75289696	-0.44336895	-1.89621062
H	-0.88763455	-2.14516472	1.60571179
H	-0.09438700	-3.19500871	0.42385176
H	-2.79842383	-0.45789990	0.35398804
H	-3.04670791	-0.79898051	-1.35599749
H	3.11794992	-1.34584591	0.85258169
H	2.21164254	-2.74968033	0.25958812
H	1.71469824	-1.96491817	1.75710277
H	-1.51700622	3.57982061	1.22328251
H	-0.47745478	3.60542423	-0.21519796
H	0.23199452	3.35302416	1.39473036
H	-1.86401300	-2.93026192	-1.17088838
N	-0.77945010	1.71200769	0.60321438
C	-0.68872251	0.95832147	1.84281484
H	-1.12131133	1.56548287	2.63617334
H	-1.25011394	0.03279130	1.79626773
H	0.34986483	0.73993355	2.10341315
F	4.06785128	0.59945276	-0.55961800
H	3.10214539	0.39525273	-0.59036581

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Ac-Pro-NMe2-exo-alpha-HFHFacceptor

optimized M062X/junccpVTZ/H2O

0 1

N	1.63069748	0.18065606	0.14721406
O	0.80573441	-0.84487307	1.95932686
O	-1.91876894	0.38923571	0.33992436
C	2.69008211	0.61322455	-0.76845891
C	2.09996876	1.87271942	-1.39900992
C	0.59911549	1.57958505	-1.44732172
C	0.35914215	0.83415084	-0.12443891
C	1.76606323	-0.61699915	1.22704214
C	3.12927873	-1.20787156	1.46461231
C	-0.85370733	-0.07794994	-0.15253448
C	-2.00479393	-2.14346555	-0.53940366
H	2.52059664	2.07855144	-2.37935494
H	0.14772692	1.54911878	0.67252219
H	2.88715289	-0.15656438	-1.51976064
H	3.61281537	0.80719593	-0.22780800
H	0.35952375	0.94118556	-2.29786449
H	-0.01606603	2.47270994	-1.51147397
H	3.05213184	-1.96615919	2.23669632
H	3.81772322	-0.42852466	1.79354999
H	3.53253663	-1.64397044	0.55122255
H	-1.67892650	-3.17534004	-0.62814560
H	-2.73931010	-1.92721009	-1.31444273
H	-2.45709086	-1.99359608	0.43679630
H	2.28982821	2.72858259	-0.75186802
N	-0.83034788	-1.28333253	-0.68183036
C	0.30257749	-1.86973452	-1.39207960
H	-0.09545677	-2.50968393	-2.17531366
H	0.91587761	-1.10990963	-1.85842499
H	0.91152254	-2.47142358	-0.71604687
F	-4.34306597	-0.09270357	-0.05975446
H	-3.40026483	0.03949905	0.07218033
F	-1.98346070	2.59235470	1.47354428
H	-1.94611154	1.73055791	1.03128882

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25 26 1.0
26 27 1.0 28 1.0 29 1.0
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30 31 1.0
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32 33 1.0
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Ac-Pro-NMe2-exo-alpha-HFHFdonor-HFHFacceptor

optimized M062X/junccpVTZ/H2O

0 1

N	-1.42752820	0.83215484	-0.06206214
O	-1.23548128	-1.34679664	-0.52984902
O	2.02870500	-0.09266946	-0.22331482
C	-2.17676163	2.07253364	0.20920666
C	-1.21862506	3.15697057	-0.27128211
C	0.16027469	2.57882130	0.04354180
C	-0.00659482	1.09245037	-0.31016844
C	-1.95633865	-0.37283324	-0.18455643
C	-3.41206080	-0.55304373	0.10523351
C	0.98209932	0.19291159	0.41492207
C	1.74494842	-1.20931716	2.19730302
H	-1.39907267	4.10699922	0.22283723
H	0.19708286	0.93792933	-1.37078755
H	-2.38170268	2.15651732	1.27836718
H	-3.12037227	2.06725824	-0.32841782
H	0.39316597	2.69596585	1.10215830
H	0.96386623	3.02705975	-0.53352183
H	-3.62633072	-1.60922116	0.23394188
H	-3.99047580	-0.17561564	-0.73968369
H	-3.70813278	0.00113655	0.99356234
H	1.25606903	-1.73585034	3.01098617
H	2.62961810	-0.69693491	2.57389875
H	2.03932489	-1.92279571	1.43279958
H	-1.32942994	3.29536971	-1.34610403
N	0.79057669	-0.24957700	1.64040291
C	-0.29328387	0.15619894	2.53002324
H	0.11332552	0.22393084	3.53580021
H	-0.68185107	1.13014156	2.26253937
H	-1.09593277	-0.58236449	2.52222831
F	4.33049093	-0.87768587	0.42725938
H	3.43514034	-0.59814350	0.23332041
F	2.52842835	1.00650654	-2.41422951
H	2.31423565	0.54563184	-1.59572111
F	-2.19185790	-3.64649845	-0.46680917
H	-1.82384865	-2.75422759	-0.49327507
F	0.35469100	-1.37215509	-2.51066266
H	-0.20952543	-1.35476082	-1.74336565

1 4 1.0 7 1.0 8 2.0
2 8 2.0
3 10 2.0
4 5 1.0 14 1.0 15 1.0
5 6 1.0 12 1.0 24 1.0
6 7 1.0 16 1.0 17 1.0
7 10 1.0 13 1.0

8 9 1.0
9 18 1.0 19 1.0 20 1.0
10 25 2.0
11 21 1.0 22 1.0 23 1.0 25 1.0
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25 26 1.0
26 27 1.0 28 1.0 29 1.0
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30 31 1.0
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32 33 1.0
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34 35 1.0
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36 37 1.0
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Ac-Pro-NMe2-exo-alpha-HFHFdonor

optimized M062X/junccpVTZ/H2O

0 1

N	0.40280152	-1.13581769	-0.06276968
O	-1.62798057	-0.24109853	0.22154694
O	0.69529585	2.11248190	1.40881935
C	1.33855745	-2.18564175	-0.50079500
C	2.52023307	-1.99764858	0.44406236
C	2.54704067	-0.48821584	0.67946972
C	1.05900513	-0.12272154	0.77681589
C	-0.89458283	-1.12850210	-0.29629126
C	-1.47315902	-2.18348824	-1.18578961
C	0.77437202	1.34555505	0.45305089
C	0.29720234	3.14718633	-1.07690922
H	3.44491583	-2.37781650	0.01942044
H	0.70980801	-0.24214171	1.80220352
H	1.62321969	-2.01967479	-1.54202096
H	0.87455287	-3.16433207	-0.41844596
H	3.01164528	0.02242402	-0.16459507
H	3.07797490	-0.19962448	1.58178758
H	-2.48566329	-1.90895660	-1.46401872
H	-1.49979313	-3.13025487	-0.64400870
H	-0.86473991	-2.32283569	-2.07749290
H	1.17497020	3.72894627	-1.36337907
H	-0.14317175	3.57842597	-0.18538531
H	-0.42359542	3.17443719	-1.89290726
H	2.32673136	-2.51897753	1.38105665
N	0.66121463	1.76098486	-0.82047824
C	0.88419549	0.95806831	-2.01163646
H	1.32358155	1.60057211	-2.77265962
H	1.58003903	0.14817299	-1.82866183
H	-0.05195435	0.55243467	-2.40295110
F	-3.99069202	-0.05047449	-0.50211394
H	-3.06686764	-0.13027308	-0.21947851

F	-1.70813552	0.23789209	2.71004096
H	-1.62602663	0.10792876	1.76813482

1 4 1.0 7 1.0 8 2.0
2 8 2.0
3 10 2.0
4 5 1.0 14 1.0 15 1.0
5 6 1.0 12 1.0 24 1.0
6 7 1.0 16 1.0 17 1.0
7 10 1.0 13 1.0
8 9 1.0
9 18 1.0 19 1.0 20 1.0
10 25 1.5
11 21 1.0 22 1.0 23 1.0 25 1.0
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25 26 1.0
26 27 1.0 28 1.0 29 1.0
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30 31 1.0
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32 33 1.0
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Ac-Pro-NMe2-exo-alpha-HFtrans

optimized M062X/junccpVTZ/H2O

0 1

N	-1.50459419	0.04192217	-0.27918103
O	-0.59879036	-1.73735238	-1.29875231
O	1.95046920	0.51218913	-0.95737077
C	-2.58756229	0.79062378	0.36510585
C	-2.16817202	2.24363631	0.15350605
C	-0.64081587	2.18081209	0.19589552
C	-0.33372488	0.86893688	-0.54193479
C	-1.55243961	-1.23516263	-0.70717436
C	-2.81465034	-2.00006545	-0.40943529
C	1.01357013	0.26795965	-0.17117242
C	2.49063399	-1.07870875	1.14348119
H	-2.58553026	2.90751615	0.90560357
H	-0.25113917	1.05061774	-1.61444082
H	-2.64749463	0.54332071	1.42890643
H	-3.54515520	0.55803074	-0.09406670
H	-0.28930744	2.13160340	1.22696714
H	-0.15766613	3.02663147	-0.28481005
H	-2.64848855	-3.04917479	-0.63044665
H	-3.63017943	-1.62753120	-1.03039126
H	-3.10957158	-1.88137705	0.63276426
H	2.37081424	-1.86905207	1.87808396
H	3.22681356	-0.35976833	1.50286482
H	2.84651697	-1.50838189	0.21018795
H	-2.49881529	2.58098199	-0.82862156
N	1.19297088	-0.44121041	0.93707164

C	0.18286513	-0.68625669	1.95918381
H	0.68470108	-0.73299520	2.92259941
H	-0.54363390	0.11522737	2.00027486
H	-0.33044177	-1.63336993	1.78204101
F	4.39168164	0.42335996	-0.84974241
H	3.41314967	0.42315378	-0.84081771

1 4 1.0 7 1.0 8 1.5
2 8 2.0
3 10 2.0
4 5 1.0 14 1.0 15 1.0
5 6 1.0 12 1.0 24 1.0
6 7 1.0 16 1.0 17 1.0
7 10 1.0 13 1.0
8 9 1.0
9 18 1.0 19 1.0 20 1.0
10 25 1.5
11 21 1.0 22 1.0 23 1.0 25 1.0
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25 26 1.0
26 27 1.0 28 1.0 29 1.0
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30 31 1.0
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Ac-Pro-NMe2-exo-alpha-thioureaacceptor

optimized M062X/junccpVTZ/H2O

0 1

N	-2.52029463	-0.62904379	0.29141991
O	-1.67698814	0.34007461	2.12955015
O	0.87161446	0.35189870	-0.19568796
C	-3.57572489	-1.26285959	-0.50316426
C	-2.78963516	-2.14826110	-1.46728656
C	-1.50147863	-1.35845456	-1.70353192
C	-1.20336028	-0.76343478	-0.31882318
C	-2.65430929	-0.08873407	1.51919559
C	-4.04909431	-0.03421673	2.08424402
C	-0.34651867	0.49472061	-0.37626468
C	0.00868024	2.85306625	-0.60085082
H	-3.33736320	-2.34991272	-2.38380068
H	-0.60366774	-1.45983319	0.26984713
H	-4.16132296	-0.50938883	-1.03774953
H	-4.24999888	-1.83086572	0.13270789
H	-1.66883744	-0.56533449	-2.43284898
H	-0.67564522	-1.97026156	-2.05554074
H	-4.04005352	0.57428730	2.98242788
H	-4.38722213	-1.04007555	2.33599646
H	-4.75028768	0.38014872	1.36047349
H	0.51805742	2.99915413	-1.55461245
H	0.75134641	2.72098832	0.18041250

H	-0.59242619	3.73116676	-0.37964807
H	-2.55931250	-3.09782288	-0.98451871
N	-0.87045796	1.69066175	-0.65132711
C	-2.25968780	1.95417191	-0.99981543
H	-2.27778730	2.78478624	-1.70201393
H	-2.71909263	1.10154113	-1.48440171
H	-2.84349821	2.22650965	-0.11828060
C	4.12101716	-0.29721857	0.16726691
N	3.68291791	0.90306421	-0.22179697
H	4.35422471	1.62392418	-0.41417813
H	2.68927449	1.07998305	-0.32522629
N	3.18599975	-1.21978342	0.40635733
H	3.47386717	-2.13426068	0.70317668
H	2.20258121	-0.99685308	0.28994022
S	5.77960422	-0.63191467	0.34803436

1 4 1.0 7 1.0 8 1.5
2 8 2.0
3 10 2.0
4 5 1.0 14 1.0 15 1.0
5 6 1.0 12 1.0 24 1.0
6 7 1.0 16 1.0 17 1.0
7 10 1.0 13 1.0
8 9 1.0
9 18 1.0 19 1.0 20 1.0
10 25 1.5
11 21 1.0 22 1.0 23 1.0 25 1.0
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25 26 1.0
26 27 1.0 28 1.0 29 1.0
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30 31 1.5 34 1.5 37 2.0
31 32 1.0 33 1.0
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34 35 1.0 36 1.0
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This structure had one negative/imaginary frequency.

Ac-Pro-NMe2-exo-alpha-ureaacceptor

optimized M062X/junccpVTZ/H2O

0 1

N	-2.14459521	-0.60782676	0.26409641
O	-1.31249491	0.33847179	2.11940318
O	1.25959472	0.34637628	-0.18069013
C	-3.19719305	-1.22650916	-0.54587813
C	-2.40866071	-2.10821329	-1.51144427
C	-1.11333823	-1.32477816	-1.72881394
C	-0.82306379	-0.74493695	-0.33614513
C	-2.28657007	-0.07815041	1.49538526
C	-3.68629417	-0.01926759	2.04793070
C	0.04740459	0.50631930	-0.37337007
C	0.38649691	2.88342469	-0.57401830
H	-2.94973803	-2.29755506	-2.43452973
H	-0.23456446	-1.45224708	0.25084859
H	-3.77247734	-0.46380556	-1.07858635
H	-3.88127918	-1.79560897	0.07844443
H	-1.26915754	-0.52378748	-2.45202681
H	-0.28856783	-1.93878521	-2.07955165
H	-3.68159524	0.58179545	2.95115640
H	-4.03305220	-1.02498408	2.28831136
H	-4.37844689	0.40534962	1.32139698
H	0.69998181	3.19499605	-1.57143942
H	1.26252196	2.66143078	0.02497981
H	-0.17326535	3.69446575	-0.11126471
H	-2.18896848	-3.06382349	-1.03566428
N	-0.47086570	1.70783614	-0.64741129
C	-1.85764671	1.97962235	-0.99645112
H	-1.86925802	2.82712342	-1.67908123
H	-2.31785610	1.14034368	-1.50318605
H	-2.44520957	2.23556655	-0.11226347
C	4.49967545	-0.55790023	0.30448637
N	4.14816586	0.71751266	-0.02003569
H	4.86654219	1.29160022	-0.42434913
H	3.18016626	0.93110626	-0.21923881
N	3.46228843	-1.36845606	0.64697395
H	3.66936240	-2.34484949	0.75893203
H	2.51569987	-1.08297708	0.43144554
O	5.67281853	-0.93190798	0.33631376

1 4 1.0 7 1.0 8 1.5
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4 5 1.0 14 1.0 15 1.0
5 6 1.0 12 1.0 24 1.0
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30 31 1.5 34 1.5 37 2.0
31 32 1.0 33 1.0
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34 35 1.0 36 1.0
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Ac-Pro-NMe2-exo-PPII-2H2Oacceptor3H2O

optimized M062X/junccpVTZ/H2O 5 H2O

0 1

N	-1.34798900	-1.27162300	-0.30358300
O	-0.86270100	-0.28971000	-2.25659500
O	0.35168700	0.78728400	0.37216100
C	-1.47472700	-2.40309500	0.62047200
C	-2.53609400	-1.91335800	1.59967100
C	-2.25395400	-0.41388100	1.68971400
C	-1.88918600	-0.03460800	0.24374500
C	-0.87453500	-1.31015900	-1.55783800
C	-0.36576500	-2.63291900	-2.05824100
C	-0.85072700	1.07900500	0.22219100
C	-0.33618400	3.44332900	0.05486900
H	-2.47162900	-2.41154100	2.56326800
H	-2.76644600	0.25159900	-0.33319400
H	-0.51999400	-2.58703200	1.11814900
H	-1.77170900	-3.30275800	0.08787800
H	-1.39243600	-0.23527200	2.33535500
H	-3.09339800	0.16623000	2.06422800
H	0.11874100	-2.48140900	-3.01755600
H	-1.19621900	-3.32909400	-2.18127500
H	0.33785800	-3.05996400	-1.34539300
H	-0.41723100	3.94843500	-0.90752600
H	0.67558000	3.08026500	0.18943400
H	-0.57433300	4.15074700	0.84760100
H	-3.52905200	-2.08344700	1.18360500
N	-1.27701500	2.33047900	0.09697300
C	-2.68287900	2.68391400	-0.09281200
H	-2.99744400	2.50064700	-1.12040400
H	-3.32416200	2.13627300	0.59179200
H	-2.79122400	3.74291100	0.12180600
H	1.15063200	-0.92632300	0.34363600
O	1.76913800	-1.67663400	0.36818500
H	2.53948800	-1.36988700	-0.13591500
O	3.00125700	1.40829500	1.22531800
H	3.43343100	0.93406100	0.49721700
H	2.05412800	1.32481200	1.03821000
O	3.76063900	-0.19882200	-1.03892600
H	3.12428400	0.18881600	-1.67397600
H	4.58012100	-0.36484600	-1.51184600
O	2.76651100	-0.90643700	2.94544900
H	2.40251500	-1.36435800	2.17150400
H	2.97292800	-0.03212800	2.58301400
O	1.61822300	1.00936400	-2.18276400
H	0.89786100	0.48553400	-2.56806100
H	1.27902200	1.16965100	-1.28852500

1 4 1.0 7 1.0 8 1.5
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36 37 1.0 38 1.0
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39 40 1.0 41 1.0
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42 43 1.0 44 1.0
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Ac-Pro-NMe2-exo-PPII-guanidinium

optimized M062X/junccpVTZ/H2O

1 1 0 1 1 1

N(Fragment=1)	-0.03092600	1.28594000	0.41143900
O(Fragment=1)	0.04913600	-0.19207400	2.09400800
O(Fragment=1)	-0.44104700	-1.15915900	-0.79555300
C(Fragment=1)	0.42969100	2.44745100	-0.35548800
C(Fragment=1)	-0.86636500	2.99312800	-0.94709700
C(Fragment=1)	-1.69616900	1.73098600	-1.18012400
C(Fragment=1)	-1.38031800	0.87224400	0.05438300
C(Fragment=1)	0.59017300	0.71307700	1.45880900
C(Fragment=1)	1.96379300	1.22944200	1.79685500
C(Fragment=1)	-1.42720400	-0.61561100	-0.27695200
C(Fragment=1)	-2.67037900	-2.69370600	-0.30572200
H(Fragment=1)	-0.69752400	3.56122900	-1.85799200
H(Fragment=1)	-2.04901500	1.09804800	0.88378900
H(Fragment=1)	1.12486300	2.13484800	-1.13852900
H(Fragment=1)	0.93344200	3.16226800	0.29055200
H(Fragment=1)	-1.34560200	1.21414400	-2.07530500
H(Fragment=1)	-2.76072000	1.92272900	-1.28679400
H(Fragment=1)	2.43315200	0.54445500	2.49561200
H(Fragment=1)	1.88411700	2.21466600	2.25841000
H(Fragment=1)	2.57928200	1.33303900	0.90275600

H(Fragment=1)	-2.95219400	-3.21038700	0.61171200
H(Fragment=1)	-1.71561200	-3.06630300	-0.65599800
H(Fragment=1)	-3.43487300	-2.87584000	-1.06064400
H(Fragment=1)	-1.36096300	3.63751900	-0.22038800
N(Fragment=1)	-2.56714400	-1.26524700	-0.04180000
C(Fragment=1)	-3.74485500	-0.64223700	0.55465000
H(Fragment=1)	-3.64327300	-0.55983500	1.63747100
H(Fragment=1)	-3.93313000	0.33923400	0.12893200
H(Fragment=1)	-4.60289900	-1.27050100	0.33186400
C(Fragment=2)	2.84510700	-1.08464900	-0.57985000
N(Fragment=2)	2.16709400	-1.76615300	0.33477800
H(Fragment=2)	2.63653000	-2.19364700	1.11429400
H(Fragment=2)	1.15392500	-1.72483100	0.32478000
N(Fragment=2)	2.17473500	-0.41276500	-1.50597000
H(Fragment=2)	2.65418700	0.04255400	-2.26308100
H(Fragment=2)	1.15693400	-0.46028000	-1.48698900
N(Fragment=1)	4.17467600	-1.06584400	-0.55650900
H(Fragment=1)	4.69671400	-0.55844400	-1.24983700
H(Fragment=1)	4.68805800	-1.60707900	0.11739300

1 4 1.0 7 1.0 8 1.5
2 8 2.0
3 10 2.0
4 5 1.0 14 1.0 15 1.0
5 6 1.0 12 1.0 24 1.0
6 7 1.0 16 1.0 17 1.0
7 10 1.0 13 1.0
8 9 1.0
9 18 1.0 19 1.0 20 1.0
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11 21 1.0 22 1.0 23 1.0 25 1.0
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30 31 1.5 34 1.5 37 1.5
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37 38 1.0 39 1.0
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Ac-Pro-NMe2-exo-PPII-H2OcisHFtrans

M062X/junccpVTZ/H2O optimized

0 1

N	-1.43415722	-0.38798508	0.17183829
O	-0.68533624	0.20459534	2.19744495

O	0.92448023	0.91196318	-0.37347931
C	-2.43702234	-0.52307924	-0.88953186
C	-1.96887885	-1.77120631	-1.62978884
C	-0.44715840	-1.68374168	-1.52050691
C	-0.22848408	-1.15772133	-0.09197005
C	-1.58472652	0.23334204	1.35818234
C	-2.89201283	0.94052469	1.59176297
C	1.01118537	-0.28168999	-0.01503966
C	3.32797590	0.04007313	0.52109865
H	-2.31588596	-1.79825513	-2.65929824
H	-0.15739905	-1.96642125	0.63428311
H	-2.42211139	0.35841956	-1.53386747
H	-3.43225239	-0.63247633	-0.46624292
H	-0.06477787	-0.95161337	-2.23334621
H	0.05730626	-2.63124555	-1.69218611
H	-2.81217764	1.53533080	2.49593853
H	-3.69056640	0.20774477	1.71525039
H	-3.13896843	1.57810197	0.74467130
H	4.03969999	-0.45683384	1.17300942
H	3.04264253	0.99063046	0.96398165
H	3.79228769	0.22409107	-0.44774131
H	-2.32965982	-2.66250601	-1.11638259
N	2.15434905	-0.81753693	0.38191822
C	2.32051293	-2.23337277	0.70245052
H	2.12018105	-2.42063184	1.75752293
H	1.67450210	-2.85318779	0.08998270
H	3.34800351	-2.50928689	0.48264701
H	-0.60131852	1.94811928	-0.66866685
O	-1.30378388	2.59756529	-0.83815657
H	-0.84286766	3.41783166	-1.03292287
F	2.51747362	2.66982205	-1.04158887
H	1.94352859	1.94068234	-0.75504375

1 4 1.0 7 1.0 8 1.5
2 8 2.0
3 10 2.0
4 5 1.0 14 1.0 15 1.0
5 6 1.0 12 1.0 24 1.0
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9 18 1.0 19 1.0 20 1.0
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30 31 1.0
31 32 1.0
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33 34 1.0
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Ac-Pro-NMe2-exo-PPII-H2Ocis

M062X/junccpVTZ/H2O optimized

0 1

N	-1.12007969	0.35368771	-0.37381619
O	-0.49645539	-1.31887108	-1.72964147
O	0.74341679	-0.98632073	1.16079310
C	-2.08362763	1.20417294	0.32813849
C	-1.33128436	2.52517024	0.44328316
C	0.11462477	2.07377114	0.64696052
C	0.24330789	0.85476091	-0.28310495
C	-1.39377283	-0.72460381	-1.13149532
C	-2.83646491	-1.14751870	-1.21156825
C	1.17498206	-0.19306232	0.32017328
C	3.39305508	-1.16256080	0.44658398
H	-1.69831084	3.14481418	1.25736502
H	0.58057413	1.13811328	-1.27897334
H	-2.30982052	0.78164522	1.30991344
H	-3.00742805	1.29086740	-0.23808158
H	0.25919910	1.75120270	1.67936566
H	0.84857118	2.84325242	0.42054634
H	-2.89253585	-2.10749464	-1.71471169
H	-3.40916622	-0.41241027	-1.77841443
H	-3.26562477	-1.22272511	-0.21398872
H	3.86662028	-1.66743127	-0.39566191
H	2.85750576	-1.88579304	1.04949221
H	4.16738533	-0.68600008	1.04834170
H	-1.42205987	3.08305899	-0.48895153
N	2.46076491	-0.16353749	-0.05322514
C	3.00618076	0.78194578	-1.01961588
H	2.83642011	0.44709862	-2.04432414
H	2.58645548	1.77469369	-0.88674872
H	4.07782595	0.85212357	-0.85073442
H	-0.94199532	-1.39136240	1.60609323
O	-1.82134300	-1.69896105	1.89984136
H	-1.64536463	-2.30393409	2.62468813

1 4 1.0 7 1.0 8 1.5
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3 10 2.0
4 5 1.0 14 1.0 15 1.0
5 6 1.0 12 1.0 24 1.0
6 7 1.0 16 1.0 17 1.0
7 10 1.0 13 1.0
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9 18 1.0 19 1.0 20 1.0
10 25 1.5
11 21 1.0 22 1.0 23 1.0 25 1.0
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25 26 1.0
26 27 1.0 28 1.0 29 1.0
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30 31 1.0
31 32 1.0
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The above structure had one negative/imaginary frequency.

Ac-Pro-NMe2-exo-PPII-HFcis

M062X/junccpVTZ/H2O optimized

0 1

N	-1.16296542	0.28818832	-0.39140577
O	-0.48842676	-1.49092821	-1.57446242
O	0.76527784	-0.90397161	1.20638690
C	-2.14717923	1.15458793	0.25983903
C	-1.42909324	2.49934770	0.29078287
C	0.03016169	2.10094428	0.50941417
C	0.18430887	0.83273931	-0.34918215
C	-1.40124377	-0.87646488	-1.02331060
C	-2.82230653	-1.37064989	-1.01382299
C	1.15385416	-0.14557578	0.29976926
C	3.39461658	-1.04528990	0.47643125
H	-1.80713337	3.15597989	1.06984162
H	0.50704113	1.06457200	-1.36285297
H	-2.36108698	0.78752009	1.26619559
H	-3.07291108	1.18330664	-0.30940344
H	0.19141379	1.84592156	1.55801496
H	0.74051233	2.87466534	0.22949132
H	-2.84697453	-2.37573650	-1.42188309
H	-3.45006651	-0.72016899	-1.62374752
H	-3.21670892	-1.36938535	0.00143948
H	3.90265361	-1.56082121	-0.33779472
H	2.88446731	-1.76591716	1.10331460
H	4.13413169	-0.50360798	1.06595529
H	-1.54102816	2.99885293	-0.67161640
N	2.42606574	-0.11232572	-0.08468117
C	2.93966758	0.78968831	-1.11138829
H	2.75882329	0.39195137	-2.11060572
H	2.50340106	1.78016961	-1.02516593
H	4.01188836	0.88552306	-0.96290106
F	-1.46793367	-1.46580501	2.01451901
H	-0.60024761	-1.18838242	1.64706434

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3 10 2.0
4 5 1.0 14 1.0 15 1.0
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6 7 1.0 16 1.0 17 1.0
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8 9 1.0
9 18 1.0 19 1.0 20 1.0
10 25 1.5
11 21 1.0 22 1.0 23 1.0 25 1.0
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25 26 1.0
26 27 1.0 28 1.0 29 1.0
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30 31 1.0
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Ac-Pro-NMe2-exo-PPII-HFdonor-HFHFacceptor

M062X/junccpVTZ/H2O optimized

0 1

N	-1.23807179	0.78075653	-0.21512183
O	-1.15564552	-1.34015743	-0.88231694
O	1.01598577	-0.24809429	0.99170853
C	-1.85150784	1.97578225	0.37744651
C	-1.05973443	3.10508172	-0.27062041
C	0.34319784	2.51247408	-0.39808516
C	0.07566641	1.04888057	-0.79004382
C	-1.78784749	-0.42629704	-0.31446169
C	-3.15176929	-0.63123357	0.26952956
C	1.12992065	0.12589959	-0.20460552
C	3.14407801	-1.17111406	-0.41234840
H	-1.07707213	4.01452752	0.32317686
H	0.01746190	0.91466542	-1.86825505
H	-1.71873137	1.95555419	1.46063664
H	-2.91283814	2.01298636	0.14868834
H	0.84777842	2.53885351	0.56879729
H	0.96666859	3.02170283	-1.12799839
H	-3.39943964	-1.68774459	0.24735259
H	-3.88845266	-0.07662544	-0.31230569
H	-3.17553377	-0.26337960	1.29377432
H	3.59999359	-1.68584291	-1.25306426
H	2.65134407	-1.89605148	0.22808869
H	3.91578922	-0.65061430	0.15395315
H	-1.46714385	3.32282151	-1.25752853
N	2.16406178	-0.22356059	-0.93986878
C	2.42088114	0.27915099	-2.28853769
H	2.03765265	-0.41747269	-3.03345712
H	1.98375504	1.25976516	-2.43649061
H	3.49683390	0.37369840	-2.40900611
F	2.74915224	-0.83161675	2.70799131
H	2.12162301	-0.62127381	2.01256624
F	-0.91767054	-0.21898214	2.56941076
H	-0.20727904	-0.18609450	1.91842285
F	-2.16186643	-3.54762330	-1.08400279
H	-1.76090933	-2.65158102	-0.99778361

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30 31 1.0
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32 33 1.0
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34 35 1.0
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Ac-Pro-NMe2-exo-PPII-HFdonor

M062X/junccpVTZ/H2O optimized

0 1

N	-0.93011007	0.88377793	-0.02525078
O	-1.23443501	-1.28472542	-0.43523378
O	0.86451982	-0.29211802	1.67402750
C	-1.33676412	2.24505494	0.33525955
C	-0.28336964	3.09296716	-0.36696817
C	0.98062312	2.24379702	-0.23251378
C	0.47512068	0.80151514	-0.41192917
C	-1.70424072	-0.19189633	-0.05065207
C	-3.13561520	-0.04787353	0.37529985
C	1.22759225	-0.16094308	0.51009157
C	3.05474690	-1.72924322	0.79345942
H	-0.17937408	4.07753988	0.08091549
H	0.52923908	0.47541960	-1.44859177
H	-1.29251021	2.37264854	1.41925215
H	-2.34847208	2.44733693	-0.00527908
H	1.39677792	2.35582753	0.76939230
H	1.75134708	2.49773750	-0.95560347
H	-3.58387078	-1.03131809	0.47487743
H	-3.68511523	0.51998073	-0.37624231
H	-3.20552990	0.48919034	1.31951216
H	3.06126177	-2.69965978	0.29544467
H	2.58789642	-1.82449552	1.76658865
H	4.08448691	-1.39160829	0.91378669
H	-0.54880848	3.21263083	-1.41725546
N	2.30628830	-0.77405699	-0.00753192
C	2.74106908	-0.62526062	-1.39031471
H	2.16754464	-1.26612159	-2.06248480
H	2.66850727	0.40630678	-1.72333010
H	3.78743660	-0.91515750	-1.44623589
F	-2.65535153	-3.24568021	-0.46726714
H	-2.08155332	-2.43714001	-0.45060825

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30 31 1.0
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Ac-Pro-NMe2-exo-PPII-HFHFacceptor

M062X/junccpVTZ/H2O optimized

0 1

N	-1.48052782	-0.33736490	0.15004882
O	-0.76643715	0.29063370	2.17674101
O	0.92322797	0.94242824	-0.31884488
C	-2.44907132	-0.45130687	-0.94409246
C	-1.97079398	-1.69809087	-1.67978608
C	-0.45253930	-1.63095496	-1.51889630
C	-0.27677810	-1.11894779	-0.07853675
C	-1.64577922	0.31674467	1.31704325
C	-2.93921123	1.06226617	1.49669688
C	0.96951412	-0.26147473	0.04665326
C	3.27161740	0.02178703	0.69954066
H	-2.28196604	-1.71096516	-2.72090713
H	-0.23659255	-1.93370716	0.64290753
H	-2.40332526	0.43606318	-1.57931572
H	-3.45852255	-0.55311245	-0.55386413
H	-0.03695581	-0.89892406	-2.21302214
H	0.04565985	-2.58335446	-1.68041100
H	-2.87771744	1.66057895	2.39978343
H	-3.76553653	0.35651368	1.58883035
H	-3.13377960	1.70140363	0.63672966
H	3.84397786	-0.41635084	1.51263999
H	2.97629706	1.02995754	0.97162874
H	3.88699396	0.05284002	-0.19914196
H	-2.35983874	-2.58954371	-1.18807902
N	2.08645013	-0.80497127	0.48526918
C	2.23449373	-2.22677071	0.79222559
H	2.02105060	-2.41705627	1.84379785
H	1.59145227	-2.83518590	0.16640397
H	3.26354116	-2.50573357	0.58239546
F	2.69867976	2.39160601	-1.31372367
H	2.05215078	1.80658753	-0.90639682

F	-1.00472704	2.45787420	-0.77608470
H	-0.31695883	1.80701314	-0.59118706

1 4 1.0 7 1.0 8 1.5
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Ac-Pro-NMe2-exo-PPII-HFHFdonor-HFHFacceptor

M062X/junccpVTZ/H2O optimized

0 1

N	-1.18780188	0.92201650	-0.25073359
O	-1.27685313	-1.27369804	-0.69264789
O	0.87953900	-0.12353908	1.20528242
C	-1.75722875	2.21400767	0.16889275
C	-0.88174442	3.21453006	-0.57263169
C	0.49292592	2.55097669	-0.54765830
C	0.17668577	1.05773826	-0.76097109
C	-1.82907991	-0.23251794	-0.24527285
C	-3.21995642	-0.27871396	0.30112050
C	1.15618992	0.19439422	0.02016228
C	3.22646093	-0.98402797	0.23672475
H	-0.88254266	4.19100777	-0.09695135
H	0.18397694	0.78636643	-1.81436726
H	-1.66374642	2.31310909	1.25155887
H	-2.80528561	2.27260604	-0.10833711
H	0.95365344	2.68468754	0.43218265
H	1.17558086	2.92950147	-1.30308969
H	-3.51488453	-1.31220856	0.45235044
H	-3.90088635	0.18378726	-0.41495046
H	-3.27726800	0.26819575	1.23900434
H	3.97212829	-1.37579845	-0.44747538
H	2.69184580	-1.81029251	0.69796021
H	3.71816424	-0.39585056	1.01072730

H	-1.23133575	3.32305831	-1.59874522
N	2.29907420	-0.15300393	-0.52969458
C	2.76102249	0.25406330	-1.85320453
H	2.81434503	-0.61844948	-2.50048055
H	2.10447461	0.99059127	-2.29779042
H	3.75047094	0.69517407	-1.74844018
F	2.16402972	-0.95463254	3.20836479
H	1.73797934	-0.65464591	2.40589436
F	-1.13627763	0.20959967	2.63687359
H	-0.38838906	0.12168188	2.03659835
F	-2.45184437	-3.45782975	-0.49484174
H	-2.00026400	-2.60670416	-0.57040510
F	0.46827506	-1.64684059	-2.45811001
H	-0.18770863	-1.48638143	-1.77687358

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Ac-Pro-NMe2-exo-PPII-HFHFdonor

M062X/junccpVTZ/H2O optimized

0 1

N	-0.90689099	1.07532329	-0.04718673
O	-1.47234534	-1.08470963	-0.27624787
O	0.65902929	-0.15111801	1.76115342
C	-1.18256867	2.49173133	0.22707072
C	-0.08497621	3.19049014	-0.56158234
C	1.11149722	2.25893405	-0.37739633
C	0.49481700	0.84554887	-0.40190546
C	-1.78438041	0.09803600	0.03535108
C	-3.17444743	0.41280944	0.49433040

C	1.16428834	-0.05211861	0.64776425
C	3.00507929	-1.50041714	1.25600203
H	0.10514525	4.19651533	-0.19808500
H	0.53654626	0.39793459	-1.39254023
H	-1.08863044	2.68101354	1.29862935
H	-2.18399117	2.75701521	-0.09760705
H	1.57162575	2.43330146	0.59603501
H	1.87375288	2.38201893	-1.14147344
H	-3.70667190	-0.51077991	0.69766065
H	-3.70020244	0.95974070	-0.28921588
H	-3.15589577	1.03480817	1.38678667
H	3.11044336	-2.49793070	0.82647341
H	2.43095741	-1.55604303	2.17292319
H	3.99984998	-1.10664371	1.46766525
H	-0.36657460	3.24391984	-1.61290957
N	2.32401865	-0.63632834	0.30638866
C	2.96676887	-0.56128892	-0.99473306
H	2.88492710	-1.52082168	-1.50606039
H	2.53201881	0.20771735	-1.62131965
H	4.02075344	-0.32338752	-0.85059740
F	-3.10210090	-2.92098490	0.03632884
H	-2.47119367	-2.19406476	-0.08507612
F	0.36990398	-2.10110072	-1.61494904
H	-0.31292128	-1.67423777	-1.08677258

1 4 1.0 7 1.0 8 1.5
2 8 2.0
3 10 2.0
4 5 1.0 14 1.0 15 1.0
5 6 1.0 12 1.0 24 1.0
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7 10 1.0 13 1.0
8 9 1.0
9 18 1.0 19 1.0 20 1.0
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11 21 1.0 22 1.0 23 1.0 25 1.0
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25 26 1.0
26 27 1.0 28 1.0 29 1.0
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30 31 1.0
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32 33 1.0
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Ac-Pro-NMe2-exo-PPII-HFtrans

M062X/junccpVTZ/H2O optimized

0 1

N	-1.55449570	-0.02300358	-0.07642740
O	-0.81300051	-1.27479186	-1.77992147
O	0.90954918	-0.80291422	0.79282304

C	-2.48637828	0.36897920	0.98021222
C	-2.18489025	1.85409989	1.14336222
C	-0.67398724	1.92168366	0.91629569
C	-0.43220631	0.89250169	-0.20376970
C	-1.65654801	-1.07708183	-0.90610077
C	-2.84550332	-1.98058845	-0.71128228
C	0.88561681	0.15691436	0.00153763
C	3.20943252	-0.16735008	-0.52068334
H	-2.48177896	2.23605519	2.11652889
H	-0.45869906	1.34804958	-1.19225685
H	-2.27459589	-0.18173642	1.90037539
H	-3.51384739	0.17475963	0.68347347
H	-0.14913142	1.60280443	1.81781721
H	-0.31992522	2.91270654	0.64419760
H	-2.72882670	-2.85509380	-1.34268237
H	-3.76155676	-1.45776933	-0.98789936
H	-2.93791547	-2.28438811	0.33078057
H	3.83013591	0.06067873	-1.38234391
H	2.99647863	-1.23266364	-0.50593347
H	3.74537255	0.09974829	0.39031342
H	-2.70671875	2.42004049	0.37165748
N	1.96602206	0.58662239	-0.63923420
C	1.99903258	1.78236295	-1.47610733
H	1.80314392	1.53575010	-2.52015098
H	1.28388496	2.52254697	-1.13370083
H	2.98999004	2.22191085	-1.39672676
F	2.68124954	-1.94332419	2.03046371
H	2.01225892	-1.46629327	1.49800955

1 4 1.0 7 1.0 8 1.5
2 8 2.0
3 10 2.0
4 5 1.0 14 1.0 15 1.0
5 6 1.0 12 1.0 24 1.0
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7 10 1.0 13 1.0
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9 18 1.0 19 1.0 20 1.0
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11 21 1.0 22 1.0 23 1.0 25 1.0
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25 26 1.0
26 27 1.0 28 1.0 29 1.0
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30 31 1.0
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Ac-Pro-NMe2-exo-PPII-thioureaacceptor

M062X/junccpVTZ/H2O optimized

0 1 0 1 0 1

N(Fragment=1)	-0.36185257	1.29485320	0.42296002
O(Fragment=1)	-0.28602653	-0.16709925	2.11919582
O(Fragment=1)	-0.64471792	-1.16567537	-0.80608375
C(Fragment=1)	0.08175489	2.46702634	-0.33675803
C(Fragment=1)	-1.21257363	2.95927258	-0.97674468
C(Fragment=1)	-1.98188480	1.66346739	-1.23225067
C(Fragment=1)	-1.68016404	0.82637486	0.02038184
C(Fragment=1)	0.24612969	0.74971211	1.49250498
C(Fragment=1)	1.58894940	1.31629713	1.86991380
C(Fragment=1)	-1.65754172	-0.66464924	-0.30271038
C(Fragment=1)	-2.81580070	-2.79212047	-0.33985692
H(Fragment=1)	-1.03420446	3.53077915	-1.88379124
H(Fragment=1)	-2.38852862	1.03340562	0.82119126
H(Fragment=1)	0.81483835	2.17498427	-1.09271808
H(Fragment=1)	0.53549746	3.20457713	0.32070920
H(Fragment=1)	-1.57313253	1.15579573	-2.10778972
H(Fragment=1)	-3.04836110	1.81055308	-1.38298955
H(Fragment=1)	2.05865469	0.65282578	2.58909321
H(Fragment=1)	1.46070121	2.30196289	2.31989788
H(Fragment=1)	2.23106889	1.42836239	0.99569633
H(Fragment=1)	-3.06865953	-3.32303217	0.57805362
H(Fragment=1)	-1.84705602	-3.12127821	-0.69537265
H(Fragment=1)	-3.57503556	-3.00890542	-1.09112783
H(Fragment=1)	-1.75890713	3.58568664	-0.27150480
N(Fragment=1)	-2.77473051	-1.36087228	-0.07663674
C(Fragment=1)	-3.98083686	-0.78312628	0.50807400
H(Fragment=1)	-3.87187208	-0.64032711	1.58392998
H(Fragment=1)	-4.23624773	0.16315553	0.03839308
H(Fragment=1)	-4.80011623	-1.47438925	0.33148766
C(Fragment=2)	2.71772338	-0.85982079	-0.48461108
N(Fragment=2)	2.01957949	-1.60038986	0.38019265
H(Fragment=2)	2.49578952	-2.00559011	1.16578924
H(Fragment=2)	1.00797393	-1.64023002	0.32411871
N(Fragment=2)	2.01281316	-0.26502572	-1.45032432
H(Fragment=2)	2.49813233	0.28227508	-2.13779313
H(Fragment=2)	1.00282260	-0.37618858	-1.48352671
S(Fragment=2)	4.40233732	-0.67792403	-0.35422760

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Ac-Pro-NMe2-exo-PPII-ureaacceptor

M062X/junccpVTZ/H2O optimized

0 1 0 1 0 1

N(Fragment=1)	0.03647567	1.25596789	0.41505827
O(Fragment=1)	0.11406025	-0.24445013	2.07810404
O(Fragment=1)	-0.48638502	-1.13790514	-0.84312147
C(Fragment=1)	0.52009329	2.40115297	-0.35978339
C(Fragment=1)	-0.77239871	3.01622024	-0.88724992
C(Fragment=1)	-1.66483391	1.79570270	-1.10911623
C(Fragment=1)	-1.33536724	0.89390280	0.09116665
C(Fragment=1)	0.67138787	0.64169959	1.42983124
C(Fragment=1)	2.07659654	1.09668202	1.72377585
C(Fragment=1)	-1.43688499	-0.58230722	-0.28362095
C(Fragment=1)	-2.75041788	-2.61747523	-0.33449965
H(Fragment=1)	-0.61534362	3.59483659	-1.79377798
H(Fragment=1)	-1.97015204	1.11506099	0.94808679
H(Fragment=1)	1.16250438	2.06436889	-1.17715921
H(Fragment=1)	1.08771041	3.08242007	0.26929762
H(Fragment=1)	-1.37405771	1.28584879	-2.02919165
H(Fragment=1)	-2.72377243	2.03447609	-1.16632542
H(Fragment=1)	2.54578726	0.37765851	2.38789409
H(Fragment=1)	2.05222800	2.07241723	2.21161637
H(Fragment=1)	2.66099761	1.19553330	0.80906147
H(Fragment=1)	-3.04032282	-3.14981732	0.57159541
H(Fragment=1)	-1.81116777	-3.01148645	-0.70353965
H(Fragment=1)	-3.52672522	-2.75799732	-1.08672609
H(Fragment=1)	-1.20747159	3.66729796	-0.12895418
N(Fragment=1)	-2.59622835	-1.20164261	-0.03533101
C(Fragment=1)	-3.73843024	-0.55896647	0.60505744
H(Fragment=1)	-3.61912178	-0.52256553	1.68888764
H(Fragment=1)	-3.89682153	0.44511456	0.22191916
H(Fragment=1)	-4.62434483	-1.14407267	0.37264021
C(Fragment=2)	2.96025998	-1.12622838	-0.59353116
N(Fragment=2)	2.20634476	-1.92016586	0.22116282
H(Fragment=2)	2.64508522	-2.20754545	1.07923967
H(Fragment=2)	1.20305531	-1.79009007	0.23125511
N(Fragment=2)	2.26469382	-0.49534132	-1.57406746
H(Fragment=2)	2.76604023	0.15534193	-2.15158443
H(Fragment=2)	1.25255727	-0.47487408	-1.53821165
O(Fragment=1)	4.18161306	-1.02588861	-0.47197768

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30 31 1.5 34 1.5 37 2.0
31 32 1.0 33 1.0
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34 35 1.0 36 1.0
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Ac-Pro-NMe2-trans-endo-alpha

optimized M062X/junccpVTZ/H2O

0 1

N	-1.14781491	0.10081904	-0.21697358
O	-0.72574282	-1.79686997	-1.34181555
O	2.24351443	0.66314331	-1.35703001
C	-1.92183305	0.94514712	0.70010738
C	-1.02647526	2.16827001	0.89272259
C	-0.26481991	2.26537341	-0.42959054
C	-0.03495839	0.80081583	-0.83582312
C	-1.43262751	-1.17314756	-0.55232538
C	-2.63700276	-1.78653501	0.11179600
C	1.39054497	0.31451306	-0.53939362
C	3.05784884	-0.98338391	0.60655194
H	-0.09631201	0.68496824	-1.91686763
H	-2.12692573	0.42150876	1.63367594
H	-2.87550386	1.22114889	0.24587364
H	0.66744912	2.81916322	-0.35570520
H	-0.88719857	2.74467796	-1.18423925
H	-2.82244350	-2.76166555	-0.32607904
H	-3.51579523	-1.15305160	-0.00350487
H	-2.45132592	-1.90116054	1.18115726
H	3.68527478	-0.35584811	1.24228720
H	3.49513162	-1.03492672	-0.38389888
H	3.00967912	-1.98176841	1.03794622
H	-1.60429607	3.06168907	1.11363362
H	-0.33225057	2.00866865	1.71767630
N	1.70394674	-0.45010130	0.52213238
C	0.84889479	-0.80865606	1.64536384
H	0.09097180	-0.06157225	1.83516888
H	0.37450912	-1.77992909	1.48839930
H	1.47650987	-0.87149476	2.53267487

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8 9 1.0
9 17 1.0 18 1.0 19 1.0

10 25 1.5
11 20 1.0 21 1.0 22 1.0 25 1.0
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26 27 1.0 28 1.0 29 1.0
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Ac-Pro-NMe2-trans-endo-PPII

optimized M062X/junccpVTZ/H2O

0 1

N	-1.34118578	0.11403892	-0.22286841
O	-1.12253088	-2.05650864	-0.75967188
O	0.63907698	-0.43198679	1.54763131
C	-2.04707319	1.26725533	0.34323341
C	-0.93897163	2.30589237	0.50679075
C	0.04477448	1.95346703	-0.60992436
C	0.02284649	0.41626035	-0.61252522
C	-1.81647228	-1.13986919	-0.31978248
C	-3.23449004	-1.35617959	0.14046620
C	1.01397403	-0.15111246	0.41380572
C	3.28887994	-0.84115686	0.90894913
H	0.21994227	-0.01116363	-1.59225378
H	-2.51925035	1.00934599	1.28950831
H	-2.81887889	1.61424051	-0.34747555
H	1.04017538	2.35917885	-0.44263813
H	-0.31987130	2.31693496	-1.57058844
H	-3.54774534	-2.35615349	-0.14081120
H	-3.90868739	-0.61918291	-0.29398520
H	-3.28848019	-1.25441642	1.22523412
H	3.76555817	-1.69713407	0.42903956
H	2.80710330	-1.16048678	1.82554653
H	4.05615860	-0.10007026	1.13742928
H	-1.31488291	3.32297455	0.43467978
H	-0.45907082	2.17923155	1.47638797
N	2.29546437	-0.27288815	0.01356865
C	2.78223784	0.04718695	-1.31914982
H	2.81504916	-0.84248870	-1.95141547
H	2.17385457	0.80521593	-1.80011243
H	3.79247311	0.44341829	-1.22830238

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4 5 1.0 13 1.0 14 1.0
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9 17 1.0 18 1.0 19 1.0
10 25 1.5
11 20 1.0 21 1.0 22 1.0 25 1.0

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26 27 1.0 28 1.0 29 1.0
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Ac-Pro-NMe2-trans-exo-alpha

optimized M062X/junccpVTZ/H2O

0 1

C	2.16804113	-0.59258437	0.61025825
H	2.00065692	-0.44857754	1.68170743
H	3.15311487	-0.20405209	0.36372738
C	1.99161451	-2.05542356	0.21189383
H	2.35773892	-2.73800811	0.97410215
C	0.48581546	-2.17355382	-0.02619652
H	-0.04317080	-2.26161018	0.92354958
H	0.20920983	-3.02190942	-0.64603609
C	0.14006210	-0.84339301	-0.71058224
H	0.27979750	-0.92824459	-1.78926324
C	1.08312511	1.39696075	-0.46855580
C	2.15999557	2.26364773	0.13037546
H	2.25823585	2.08373519	1.20068319
H	1.91143515	3.30446919	-0.04873911
H	3.12139477	2.03971262	-0.33318843
C	-1.32700833	-0.44710811	-0.56418255
C	-3.19125737	0.50301085	0.57343117
H	-3.85211534	-0.34144561	0.38498525
H	-3.35743544	1.24633771	-0.20638674
H	-3.42948301	0.93881179	1.53857775
N	1.12892522	0.08513804	-0.16946501
O	0.19470022	1.85375652	-1.18646492
O	-2.07506332	-0.67012937	-1.51517463
H	2.53005740	-2.24977196	-0.71570114
N	-1.79735395	0.07451496	0.58380273
C	-1.00636710	0.38405627	1.76489073
H	-0.21070562	-0.33780897	1.90898119
H	-0.57429740	1.38651086	1.71318578
H	-1.65665415	0.33158654	2.63457340

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Ac-Pro-NMe2-trans-exo-PPII

optimized M062X/junccpVTZ/H2O

0 1

N	-1.31435744	0.00651903	-0.08182152
O	-0.63224618	-1.99972068	-0.81389065
O	0.80928757	-0.48855813	1.60125889
C	-2.28652552	0.97565649	0.42201928
C	-1.70845129	2.29911413	-0.06643130
C	-0.20095161	2.07604933	0.05566275
C	-0.01622491	0.60421979	-0.35662148
C	-1.52278460	-1.29616772	-0.33594419
C	-2.89184288	-1.84068290	-0.01929634
C	1.07617093	-0.06183550	0.48225460
C	3.40003353	-0.73376886	0.67617311
H	-2.05806813	3.14752781	0.51631255
H	0.19627274	0.50384758	-1.41943347
H	-2.32987947	0.94201376	1.51391576
H	-3.27818978	0.77339323	0.02540865
H	0.10734991	2.19846699	1.09490813
H	0.38919317	2.75034556	-0.56013784
H	-2.87071413	-2.92063199	-0.12226590
H	-3.62658006	-1.42971895	-0.71264535
H	-3.19905922	-1.56932723	0.98992584
H	3.80573942	-1.54914092	0.07555291
H	3.02292788	-1.12721140	1.61261865
H	4.19758782	-0.01736741	0.87487815
H	-1.98275300	2.45530544	-1.10985953
N	2.31524762	-0.08612862	-0.04310855
C	2.64311376	0.41866017	-1.37018841
H	2.35532173	-0.28598627	-2.15273413
H	2.17361517	1.38063563	-1.55944249
H	3.71944912	0.56387603	-1.41720550

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Coordinates of structures of Ac-Ala-NMe_2 as a function of ring pucker, main chain conformation, and explicit solvation

Ac-Ala-NMe2-alpha-H2OH2OacceptorH2OH2O

optimized M062X/junccpVTZ/H2O

0 1

N	-2.00300000	-0.80700000	0.16200000
O	-1.17600000	-0.65300000	2.24800000
O	1.39400000	0.15600000	0.04700000
C	-0.78900000	-1.13000000	-1.93800000
C	-0.69000000	-0.86100000	-0.44000000
C	-2.14600000	-0.69600000	1.49600000
C	-3.56000000	-0.61500000	2.00800000
C	0.18800000	0.36100000	-0.16200000
C	0.58000000	2.69000000	0.21500000
H	-0.13300000	-1.67300000	0.02800000
H	-1.32900000	-0.33800000	-2.45500000
H	0.21100000	-1.20600000	-2.36200000
H	-3.70000000	0.35500000	2.48400000
H	-3.70200000	-1.38300000	2.76700000
H	-4.29900000	-0.73900000	1.22100000
H	-0.02700000	3.53800000	0.52000000
H	1.21100000	2.98400000	-0.62600000
H	1.21600000	2.38500000	1.04100000
N	-0.31100000	1.59700000	-0.16000000
C	-1.65100000	1.98400000	-0.58500000
H	-1.56800000	2.90700000	-1.15600000
H	-2.10300000	1.23400000	-1.22200000
H	-2.29700000	2.16100000	0.27600000
H	2.98700000	1.10900000	0.05100000
H	2.38300000	-1.38000000	-0.20600000
H	-2.81700000	-0.76600000	-0.44100000
H	-1.31000000	-2.07100000	-2.10600000
O	2.98200000	-2.12900000	-0.35800000
O	3.87600000	1.49700000	0.05600000
H	3.86800000	-1.78000000	-0.19000000
H	4.48000000	0.74400000	0.10100000
O	5.57500000	-0.87900000	0.15000000
H	6.25300000	-0.96100000	-0.52800000
H	6.01500000	-1.08100000	0.98100000
O	-4.08900000	-0.36400000	-1.84700000
H	-4.92600000	0.07100000	-1.65700000
H	-4.30400000	-1.06900000	-2.46600000

1 5 1.0 6 1.5 26 1.0
2 6 2.0
3 8 2.0
4 5 1.0 11 1.0 12 1.0 27 1.0
5 8 1.0 10 1.0
6 7 1.0
7 13 1.0 14 1.0 15 1.0
8 19 1.5
9 16 1.0 17 1.0 18 1.0 19 1.0
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19 20 1.0
20 21 1.0 22 1.0 23 1.0

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24 29 1.0
25 28 1.0
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28 30 1.0
29 31 1.0
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32 33 1.0 34 1.0
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35 36 1.0 37 1.0
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Ac-Ala-NMe2-alpha-HFdonor-HFHFacceptor

optimized M062X/junccpVTZ/H2O

0 1

N	-1.33467400	-1.06883700	0.87438000
O	-1.64594500	0.97165400	0.03951800
O	1.71257000	0.59701500	0.22684400
C	0.71082200	-1.96372300	1.90031400
C	0.05062500	-0.78416700	1.19709100
C	-2.12196200	-0.13768500	0.33186400
C	-3.55655300	-0.48016400	0.07718900
C	0.87973500	-0.32265300	0.00109000
C	1.49866200	-0.25649700	-2.31464900
H	0.06426300	0.07516700	1.86758100
H	0.73136200	-2.85320300	1.27308100
H	1.73363100	-1.70082200	2.16186800
H	-3.73633100	-0.43007200	-0.99618900
H	-4.18234200	0.27103800	0.55599300
H	-3.82071500	-1.46709500	0.44455600
H	0.96468100	-0.49364800	-3.23027300
H	2.50869600	-0.66154500	-2.36837000
H	1.54620200	0.82134200	-2.19376100
N	0.76448400	-0.85189700	-1.19796100
C	-0.00974200	-2.04453000	-1.53373300
H	0.58845500	-2.64375900	-2.21658300
H	-0.22402000	-2.64159300	-0.65824200
H	-0.94100900	-1.76563400	-2.02671700
F	3.90461000	1.17056100	-0.85625100
H	3.05253800	0.92877300	-0.48745600
F	1.78144200	1.79420600	2.40191200
H	1.75201800	1.32877100	1.55437600
F	-3.15065300	2.61913100	-0.97640500
H	-2.54940800	1.96268600	-0.56980500
H	-1.72542400	-1.96233300	1.13026700
H	0.16762600	-2.19085100	2.81555100

1 5 1.0 6 1.5 30 1.0
2 6 2.0
3 8 2.0
4 5 1.0 11 1.0 12 1.0 31 1.0
5 8 1.0 10 1.0
6 7 1.0
7 13 1.0 14 1.0 15 1.0
8 19 2.0
9 16 1.0 17 1.0 18 1.0 19 1.0
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20 21 1.0 22 1.0 23 1.0
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24 25 1.0
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26 27 1.0
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28 29 1.0
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Ac-Ala-NMe2-alpha-HFHFacceptor

optimized M062X/junccpVTZ/H2O

0 1

N	1.85267209	-0.44730752	0.55837208
O	1.51747460	-0.44775634	-1.65616244
O	-1.57802689	-0.42191778	-0.27534777
C	0.23541340	-0.99435581	2.32264201
C	0.48328946	-0.82238046	0.82835364
C	2.28914069	-0.31337335	-0.71396833
C	3.74472920	0.01491989	-0.90052243
C	-0.54619069	0.12003321	0.21082177
C	-1.36354247	2.24591157	-0.54416659
H	0.28727459	-1.77369038	0.33197159
H	0.40130176	-0.06901402	2.87197534
H	-0.79100411	-1.31578194	2.48686898
H	3.82004587	0.91836366	-1.50284802
H	4.21303778	-0.79759433	-1.45373970
H	4.26877950	0.15974876	0.04024099
H	-0.86485871	3.16535926	-0.83717023
H	-2.22598338	2.48421400	0.07740406
H	-1.69302495	1.71654161	-1.43297135
N	-0.40247337	1.42819396	0.19560909
C	0.64669226	2.17448461	0.88548159
H	0.19645388	3.07864468	1.28862476
H	1.06328499	1.60635205	1.70549600
H	1.43882424	2.45026097	0.18915023
F	-3.92748573	0.41326869	-0.50873398
H	-3.00962578	0.14080550	-0.42281007
F	-1.78538299	-2.87944605	-0.52602998
H	-1.69366951	-1.91985173	-0.42717933
H	2.49698106	-0.34997419	1.32632845
H	0.90383747	-1.75903796	2.71389735

1 5 1.0 6 1.5 28 1.0
2 6 2.0
3 8 2.0
4 5 1.0 11 1.0 12 1.0 29 1.0
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7 13 1.0 14 1.0 15 1.0
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20 21 1.0 22 1.0 23 1.0
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24 25 1.0
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26 27 1.0
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Ac-Ala-NMe2-alpha-HFHFdonor-HFacceptor

optimized M062X/junccpVTZ/H2O

0 1

N	1.03502097	-1.36960952	-0.66080304
O	1.63610592	0.69761902	-0.05000763
O	-1.80193391	0.72641965	-0.65586807
C	-0.96316351	-2.11271925	-1.87069982
C	-0.24516121	-0.94383925	-1.20829129
C	1.89660994	-0.52844524	-0.11142311
C	3.16931800	-1.06636643	0.45568646
C	-1.15158038	-0.23119112	-0.20062378
C	-1.99838151	0.20661344	2.00308599
H	-0.05702322	-0.17856740	-1.96039154
H	-1.17584235	-2.91230838	-1.16310881
H	-1.90343938	-1.76230886	-2.28986165
H	3.20471045	-0.81565916	1.51550708
H	4.00383035	-0.56638890	-0.03358576
H	3.25787497	-2.14097178	0.33099653
H	-1.59029646	0.05206617	2.99840411
H	-3.05157020	-0.07476647	1.99697549
H	-1.90622731	1.25498032	1.73632932
N	-1.23473530	-0.61462319	1.06742881
C	-0.69387744	-1.84964046	1.62567612
H	-1.42878967	-2.24882424	2.32147690
H	-0.52571761	-2.59574990	0.85999649
H	0.23392363	-1.65991832	2.16630076
F	-3.88604820	1.82111719	0.05241832
H	-3.05393639	1.37087992	-0.17910658
F	3.24489460	2.11083011	1.23510925
H	2.62157022	1.57028643	0.73569345
F	0.86280269	2.24168497	-1.93081494
H	1.08509695	1.65226996	-1.21891690
H	1.28298680	-2.34690010	-0.70960748
H	-0.34995175	-2.50996022	-2.67735315

1 5 1.0 6 1.5 30 1.0
2 6 2.0
3 8 2.0
4 5 1.0 11 1.0 12 1.0 31 1.0
5 8 1.0 10 1.0
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7 13 1.0 14 1.0 15 1.0
8 19 2.0
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28 29 1.0
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Ac-Ala-NMe2-alpha-HFHFdonor-HFHFacceptor

optimized M062X/junccpVTZ/H2O

0 1

N	-1.23702879	-0.57472389	1.38841944
O	-1.74469603	0.71502548	-0.36818657
O	1.77157071	0.39552964	-0.22555396
C	0.89061652	-0.80982418	2.58842694
C	0.16312391	-0.18069641	1.40570657
C	-2.10910239	-0.10059230	0.51086301
C	-3.52441072	-0.57400127	0.57529226
C	0.90586578	-0.45806522	0.09895039
C	1.32471106	-1.62042281	-1.95456684
H	0.20608603	0.90421246	1.50789981
H	0.89202766	-1.89707218	2.52926804
H	1.92015098	-0.45922432	2.60241102
H	-3.79061206	-0.99643782	-0.39279555
H	-4.16672851	0.28801063	0.75174341
H	-3.67938044	-1.31362917	1.35460751
H	0.71236223	-2.25933643	-2.58401734
H	2.31907700	-2.05417694	-1.85290360
H	1.40257148	-0.63714360	-2.40781681
N	0.67329578	-1.51716809	-0.64803272
C	-0.12714293	-2.67639043	-0.25679899
H	0.37528708	-3.56225831	-0.63766753
H	-0.19473146	-2.76826291	0.81925699
H	-1.12512033	-2.62176249	-0.69099301
F	3.82858971	0.27633556	-1.67653206
H	3.02807490	0.27817973	-1.15176173
F	2.45402281	2.14186854	1.43115158
H	2.15436429	1.51643898	0.76336831
F	-3.47410761	1.32468500	-2.07238472
H	-2.80259678	1.09990686	-1.42038147
F	-0.22507683	2.75815646	-0.21187162
H	-0.75282301	1.97040647	-0.27470751
H	-1.56777220	-1.21347797	2.09630414
H	0.40807675	-0.50502429	3.51489389

1 5 1.0 6 1.5 32 1.0
2 6 2.0
3 8 2.0
4 5 1.0 11 1.0 12 1.0 33 1.0
5 8 1.0 10 1.0
6 7 1.0
7 13 1.0 14 1.0 15 1.0

8 19 2.0
9 16 1.0 17 1.0 18 1.0 19 1.0
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20 21 1.0 22 1.0 23 1.0
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24 25 1.0
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26 27 1.0
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28 29 1.0
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30 31 1.0
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Ac-Ala-NMe2-alpha-HFHFdonor

optimized M062X/junccpVTZ/H2O

0 1

N	0.12239532	-0.61348177	-1.37149500
O	1.56049231	0.22259808	0.12879411
O	-1.59831947	1.72941430	0.64332304
C	-1.96787937	0.33419878	-2.22836622
C	-0.85016709	0.45941038	-1.20125182
C	1.25437289	-0.67747707	-0.69191764
C	2.15699048	-1.85002723	-0.90023865
C	-1.40515515	0.59147202	0.22626154
C	-2.07138562	-0.31315151	2.35048265
H	-0.33756474	1.40717965	-1.35924743
H	-2.51855470	-0.59911317	-2.12014184
H	-2.66391025	1.15976529	-2.09932432
H	2.29113757	-2.35246656	0.05727656
H	3.13023668	-1.48414827	-1.22406957
H	1.76605607	-2.55232774	-1.62987939
H	-3.15839271	-0.25437352	2.43283481
H	-1.63706984	0.60162956	2.73916792
H	-1.71885035	-1.16221980	2.93253535
N	-1.66325034	-0.50085117	0.96527494
C	-1.71349413	-1.87532079	0.48878000
H	-2.57544788	-2.35979233	0.94527621
H	-1.84353878	-1.92544241	-0.58507699
H	-0.81541662	-2.42775356	0.77091060
F	3.60977114	-0.16026813	1.49184999
H	2.81559331	-0.00758521	0.96314777
F	1.51377311	2.74787354	-0.17064344
H	1.45677331	1.80547702	-0.04542214
H	-0.07926242	-1.35083257	-2.03029713
H	-1.55477670	0.38315895	-3.23444538

1 5 1.0 6 2.0 28 1.0
2 6 2.0
3 8 2.0
4 5 1.0 11 1.0 12 1.0 29 1.0
5 8 1.0 10 1.0

6 7 1.0
7 13 1.0 14 1.0 15 1.0
8 19 1.5
9 16 1.0 17 1.0 18 1.0 19 1.0
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20 21 1.0 22 1.0 23 1.0
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24 25 1.0
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26 27 1.0
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Ac-Ala-NMe2-alpha-HFtrans

optimized M062X/junccpVTZ/H2O

0 1

N	-1.76256800	0.66558100	0.08478800
O	-1.44525600	-0.79213900	-1.59001600
O	1.61709100	0.55686300	-0.89417200
C	-0.28413300	2.46633900	0.84507700
C	-0.47707500	1.29923300	-0.11583800
C	-2.17052200	-0.34977700	-0.70663600
C	-3.53911100	-0.91201800	-0.43334300
C	0.71417100	0.34163600	-0.06173200
C	1.89241500	-1.59669100	0.71344000
H	-0.43346200	1.67605700	-1.13782600
H	-0.30795100	2.14580500	1.88585500
H	0.67619500	2.94009700	0.65303800
H	-3.43057200	-1.96023000	-0.15857600
H	-4.12204900	-0.86587300	-1.35116900
H	-4.06456400	-0.38514700	0.35861800
H	1.60043900	-2.51350000	1.21801400
H	2.79821900	-1.20342700	1.17529900
H	2.09395200	-1.81128700	-0.33247900
N	0.79175200	-0.64413800	0.82387000
C	-0.11233900	-0.85537000	1.94823700
H	0.48581800	-1.15217400	2.80744500
H	-0.64546600	0.04953200	2.20622100
H	-0.82925300	-1.64668200	1.72548900
F	3.98670600	-0.03219300	-1.02454400
H	3.03115000	0.15983500	-0.93327800
H	-2.38217400	1.02519000	0.79254800
H	-1.07003100	3.20354100	0.68936500

1 5 1.0 6 1.5 26 1.0
2 6 2.0
3 8 2.0
4 5 1.0 11 1.0 12 1.0 27 1.0
5 8 1.0 10 1.0
6 7 1.0
7 13 1.0 14 1.0 15 1.0
8 19 1.5
9 16 1.0 17 1.0 18 1.0 19 1.0

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20 21 1.0 22 1.0 23 1.0
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24 25 1.0
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Ac-Ala-NMe2-alpha

optimized M062X/junccpVTZ/H2O

0 1

N	-1.26415200	0.65114200	0.32888100
O	-1.46500900	-0.71031400	-1.44560000
O	1.76823800	0.60031000	-1.49081200
C	0.36054100	2.43542000	0.73257200
C	-0.07348300	1.29789500	-0.18368200
C	-1.89246900	-0.32053400	-0.36443900
C	-3.12837400	-0.90625600	0.26561800
C	1.10157400	0.35627800	-0.48663500
C	2.43183300	-1.60859100	-0.05324600
H	-0.30602800	1.70949200	-1.16582100
H	0.61696700	2.07983600	1.73002500
H	1.23368900	2.92698400	0.30878500
H	-2.94757100	-1.96262100	0.45948800
H	-3.94859600	-0.83210900	-0.44569400
H	-3.40560900	-0.41319700	1.19357100
H	3.36849100	-1.38010500	0.45901900
H	2.58994200	-1.55776800	-1.12458100
H	2.11841700	-2.61416800	0.22402400
N	1.38814100	-0.67131400	0.33265000
C	0.78738300	-0.92835600	1.63241800
H	1.56553200	-1.30630900	2.29423700
H	0.38690800	-0.02523200	2.07490300
H	-0.00454700	-1.67694900	1.56378500
H	-1.64292000	0.95019400	1.21279700
H	-0.44046600	3.16804900	0.82040700

1 5 1.0 6 1.5 24 1.0
2 6 2.0
3 8 2.0
4 5 1.0 11 1.0 12 1.0 25 1.0
5 8 1.0 10 1.0
6 7 1.0
7 13 1.0 14 1.0 15 1.0
8 19 1.5
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Ac-Ala-NMe2-alpha-ureaacceptor

optimized M062X/junccpVTZ/H2O

0 1 0 1 0 1

N(Fragment=1)	1.93191400	-1.09727300	0.59927800
O(Fragment=1)	2.42141100	-0.80802300	-1.57121500
O(Fragment=1)	-0.69055000	0.65236700	-1.01562500
C(Fragment=1)	-0.24930400	-0.95413600	1.70678400
C(Fragment=1)	0.53175000	-0.78451800	0.40919300
C(Fragment=1)	2.79214200	-1.10426500	-0.44098000
C(Fragment=1)	4.21786200	-1.47868200	-0.13728500
C(Fragment=1)	0.24997400	0.58850000	-0.21162000
C(Fragment=1)	0.70904900	2.92748700	-0.55822100
H(Fragment=1)	0.13005800	-1.47367800	-0.33462900
H(Fragment=1)	0.10609400	-0.27967300	2.48500800
H(Fragment=1)	-1.30284200	-0.74575000	1.52566600
H(Fragment=1)	4.86056200	-0.65081000	-0.43222800
H(Fragment=1)	4.48531700	-2.34242500	-0.74341300
H(Fragment=1)	4.38318300	-1.70784000	0.91205100
H(Fragment=1)	0.06485300	3.57161800	0.04238800
H(Fragment=1)	0.23499400	2.73509300	-1.51357400
H(Fragment=1)	1.66174200	3.43047400	-0.71520900
N(Fragment=1)	0.95883300	1.66804200	0.13092800
C(Fragment=1)	1.95282200	1.74403300	1.19305000
H(Fragment=1)	1.85400500	2.71723200	1.67103800
H(Fragment=1)	1.79523100	0.98415200	1.94747500
H(Fragment=1)	2.96372200	1.65226900	0.79251800
C(Fragment=2)	-3.82364000	-0.45676700	-0.12000600
N(Fragment=2)	-3.45660200	0.84021100	0.07253600
H(Fragment=2)	-3.96015600	1.36023700	0.76876400
H(Fragment=2)	-2.53507500	1.14821200	-0.20348100
N(Fragment=2)	-2.99738100	-1.16749400	-0.93433700
H(Fragment=2)	-3.15905100	-2.15695900	-0.99579100
H(Fragment=2)	-2.08246000	-0.79658800	-1.15835200
O(Fragment=1)	-4.84883500	-0.93274700	0.36775100
H(Fragment=1)	2.25871300	-1.35393500	1.51662800
H(Fragment=1)	-0.15636600	-1.97872300	2.06352100

1 5 1.0 6 1.5 32 1.0
2 6 2.0
3 8 2.0
4 5 1.0 11 1.0 12 1.0 33 1.0
5 8 1.0 10 1.0
6 7 1.0
7 13 1.0 14 1.0 15 1.0
8 19 1.5
9 16 1.0 17 1.0 18 1.0 19 1.0
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19 20 1.0

20 21 1.0 22 1.0 23 1.0
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24 25 1.5 28 1.5 31 2.0
25 26 1.0 27 1.0
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28 29 1.0 30 1.0
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Ac-Ala-NMe2-beta-H2OH2OacceptorH2OH2O

optimized M062X/junccpVTZ/H2O 4 H2O

0 1

N	-1.73300000	-0.64500000	-0.17900000
O	-3.97500000	-0.42700000	-0.34900000
O	0.73700000	0.31600000	-0.30100000
C	-1.72500000	0.82400000	1.79600000
C	-1.54600000	0.71300000	0.27800000
C	-2.96600000	-1.12500000	-0.43000000
C	-3.03900000	-2.58200000	-0.80500000
C	-0.14300000	1.16900000	-0.09400000
C	1.51800000	2.85800000	-0.39800000
H	-2.29500000	1.31900000	-0.22600000
H	-0.97900000	0.20900000	2.29900000
H	-1.61800000	1.85300000	2.13900000
H	-2.08300000	-2.96800000	-1.15100000
H	-3.79800000	-2.71000000	-1.57200000
H	-3.34700000	-3.14800000	0.07500000
H	1.61800000	3.92400000	-0.21600000
H	1.78400000	2.64200000	-1.43300000
H	2.19600000	2.31300000	0.25500000
N	0.13700000	2.47000000	-0.12800000
C	-0.81300000	3.55700000	0.06000000
H	-0.79600000	4.20700000	-0.81500000
H	-1.82100000	3.18600000	0.19500000
H	-0.53400000	4.14000000	0.93700000
H	2.41200000	0.25300000	-1.17700000
H	1.69500000	-0.70400000	0.92400000
H	-0.93900000	-1.27900000	-0.18500000
H	-2.71700000	0.46500000	2.06300000
O	2.08500000	-1.45500000	1.40000000
O	3.27100000	0.12600000	-1.60700000
H	3.00800000	-1.50500000	1.11000000
H	3.79300000	-0.41000000	-0.99600000
O	4.72900000	-1.52600000	0.31700000
H	5.04000000	-2.38200000	0.00400000
H	5.46700000	-1.14100000	0.80000000
O	0.22600000	-2.94800000	-0.00700000
H	-0.15300000	-3.65300000	0.52400000
H	0.94200000	-2.56200000	0.53500000

1 5 1.0 6 1.5 26 1.0
2 6 2.0
3 8 2.0
4 5 1.0 11 1.0 12 1.0 27 1.0
5 8 1.0 10 1.0
6 7 1.0
7 13 1.0 14 1.0 15 1.0
8 19 1.5
9 16 1.0 17 1.0 18 1.0 19 1.0

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19 20 1.0
20 21 1.0 22 1.0 23 1.0
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24 29 1.0
25 28 1.0
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28 30 1.0
29 31 1.0
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32 33 1.0 34 1.0
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35 36 1.0 37 1.0
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Ac-Ala-NMe2-beta-HFdonor-HFHFacceptor

fixed phi optimized M062X/junccpVTZ/H2O

0 1

N	0.98267600	0.49884600	0.00113000
O	2.84657000	-0.72734500	-0.20825800
O	-1.70015300	0.81332000	-0.01010300
C	0.30295200	-1.05311000	1.79386400
C	0.17083600	-0.66272800	0.31734600
C	2.29701700	0.38749700	-0.19350900
C	3.07705000	1.64914000	-0.40669600
C	-1.28828000	-0.37775900	0.00734200
C	-3.54347000	-1.08276400	-0.36901900
H	0.53433300	-1.46810100	-0.31404800
H	-0.04547400	-0.23695300	2.42593900
H	-0.28199100	-1.94368700	2.01717400
H	3.58978600	1.58028800	-1.36489200
H	3.83456200	1.72324300	0.37234900
H	2.44899200	2.53505100	-0.39042100
H	-3.71113600	-0.64034100	-1.34979300
H	-3.88766200	-0.39450700	0.39915100
H	-4.09561700	-2.01355700	-0.29419200
N	-2.12225100	-1.37878700	-0.17842300
C	-1.76585400	-2.79450800	-0.21377500
H	-2.11433100	-3.21935700	-1.15312500
H	-0.69781100	-2.94637300	-0.13439000
H	-2.25842500	-3.30464700	0.61241100
H	0.59288500	1.42370000	0.10960200
H	1.34854200	-1.25449900	2.01498300
F	-3.71985900	2.01327800	-0.95792900
H	-2.99228300	1.49857100	-0.61672800
F	-0.65415300	2.81759200	1.01950300
H	-1.11971400	2.05075500	0.66826900
F	5.24934000	-0.78128100	-0.63528500
H	4.28158300	-0.75870300	-0.46427600

1 5 1.0 6 1.5 24 1.0

2 6 2.0
3 8 2.0
4 5 1.0 11 1.0 12 1.0 25 1.0
5 8 1.0 10 1.0
6 7 1.0
7 13 1.0 14 1.0 15 1.0
8 19 2.0
9 16 1.0 17 1.0 18 1.0 19 1.0
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19 20 1.0
20 21 1.0 22 1.0 23 1.0
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Attempted optimization of the above structure without phi fixed led to geometry optimization with a PPII conformation. Despite the use of a fixed value of phi, frequency calculations on this structure resulted in no observed imaginary/negative frequencies.

Ac-Ala-NMe2-beta-HFHFacceptor

fixed phi optimized M062X/jun-cc-pVTZ/H2O

0 1

N	1.50670000	0.19405500	-0.16255300
O	3.11127100	-1.31730500	-0.65059700
O	-1.08452400	0.94540700	0.08239900
C	0.71922100	-1.33706700	1.60861000
C	0.53930600	-0.82993200	0.17218700
C	2.77670800	-0.15147800	-0.48198600
C	3.74980000	0.98713500	-0.63677200
C	-0.87316100	-0.29650000	0.01139600
C	-3.24154000	-0.60600700	-0.17859500
H	0.71031900	-1.64295500	-0.52776500
H	0.56305300	-0.52040100	2.31324900
H	0.01529400	-2.13592000	1.83717400
H	3.28409500	1.96242500	-0.52034000
H	4.20947100	0.91726700	-1.62069400
H	4.53483600	0.87022100	0.10879000
H	-3.93020200	-1.43087400	-0.02810500
H	-3.43961800	-0.14099500	-1.14333200
H	-3.38012100	0.12971100	0.60913400
N	-1.87777200	-1.13538000	-0.13655600
C	-1.76620000	-2.58369200	-0.27963300
H	-2.26129200	-2.88349500	-1.20147300
H	-0.73512400	-2.90849400	-0.31219400
H	-2.26244500	-3.06371200	0.56242400
H	-2.25102200	1.83861700	-0.48075800
H	-0.25100300	2.00002600	0.77200600
H	1.33486700	1.14579200	0.12401500

H	1.73217500	-1.71655700	1.72215200
F	0.34957900	2.65266800	1.15622600
F	-2.89564100	2.46389400	-0.80802400

1 5 1.0 6 1.5 26 1.0
2 6 2.0
3 8 2.0
4 5 1.0 11 1.0 12 1.0 27 1.0
5 8 1.0 10 1.0
6 7 1.0
7 13 1.0 14 1.0 15 1.0
8 19 2.0
9 16 1.0 17 1.0 18 1.0 19 1.0
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19 20 1.0
20 21 1.0 22 1.0 23 1.0
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24 29 1.0
25 28 1.0
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Attempted optimization of the above structure without phi fixed led to geometry optimization with a PPII conformation. Despite the use of a fixed value of phi, frequency calculations on this structure resulted in no observed imaginary/negative frequencies.

Ac-Ala-NMe2-beta-HFHFdonor-HFacceptor

optimized M062X/junccpVTZ/H2O

0 1

N	-0.66547247	-0.90869337	0.18606078
O	-2.65846540	0.08369109	-0.13597141
O	1.90756443	-1.18647156	0.14804267
C	-0.05644016	0.94381425	1.68659723
C	0.08543291	0.33050817	0.29104406
C	-1.96759807	-0.96048166	-0.01002988
C	-2.62443362	-2.30078573	-0.08532263
C	1.54652998	-0.00165992	0.02035215
C	3.80259866	0.63691998	-0.43077036
H	-0.29012212	1.01127506	-0.46806363
H	0.35041141	0.25878590	2.42940491
H	0.47556066	1.89081791	1.74971379
H	-3.12762479	-2.38507210	-1.04748347
H	-3.38228866	-2.35964213	0.69470225
H	-1.91435921	-3.11330057	0.03038659
H	3.94731564	-0.03034300	-1.27905303
H	4.17144554	0.14804234	0.46913422
H	4.35670699	1.55513880	-0.59505799
N	2.38844678	0.97431971	-0.28045704
C	2.03337188	2.37720977	-0.46115907
H	2.40877591	2.71499107	-1.42528439
H	0.96068359	2.52672162	-0.43717365

H	2.49136946	2.97457321	0.32666242
H	-0.13334275	-1.76339793	0.28458365
H	-1.10727161	1.12173480	1.90411966
F	3.98010997	-2.50769519	-0.15545964
H	3.20200909	-1.94288826	-0.04826931
F	-5.10023722	-0.23192572	-0.50814765
H	-4.15339039	-0.10413919	-0.36385205
F	-2.09419034	2.53016550	-0.17784134
H	-2.29740227	1.59151131	-0.15149755

1 5 1.0 6 1.5 24 1.0
2 6 2.0
3 8 2.0
4 5 1.0 11 1.0 12 1.0 25 1.0
5 8 1.0 10 1.0
6 7 1.0
7 13 1.0 14 1.0 15 1.0
8 19 1.5
9 16 1.0 17 1.0 18 1.0 19 1.0
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26 27 1.0
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28 29 1.0
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30 31 1.0
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Ac-Ala-NMe2-beta-HFHFdonor-HFHFacceptor

optimized M062X/junccpVTZ/H2O

0 1

N	-0.73872341	-0.80027066	0.19454348
O	-2.69679389	0.20782922	-0.29200654
O	1.96770150	-0.86915736	0.03029175
C	-0.14539375	0.91550473	1.85839116
C	-0.01875612	0.44379558	0.40725519
C	-2.02466762	-0.83783738	-0.11322709
C	-2.67499327	-2.17640942	-0.25229791
C	1.44684251	0.27824347	0.04144505
C	3.60521889	1.19589046	-0.44085579
H	-0.45976622	1.17162578	-0.26536829
H	0.30074955	0.18139084	2.52850100
H	0.35245724	1.87260926	2.00104127
H	-3.10792883	-2.24834240	-1.24900791
H	-3.48682683	-2.24287889	0.47069164
H	-1.97573974	-2.99221734	-0.09634968
H	3.78701225	0.83988083	-1.45401408
H	4.02431996	0.48993514	0.27069174
H	4.07489325	2.16511919	-0.30873788
N	2.16881651	1.35045145	-0.20377059
C	1.66930654	2.72146410	-0.28111183

H	1.96997364	3.14442540	-1.23762465
H	0.59061091	2.77178069	-0.19897950
H	2.11471927	3.30666680	0.52200011
H	-0.28554767	-1.67817630	0.41381530
H	-1.19840144	1.03146881	2.10663246
F	3.94893671	-1.85357574	-1.21162071
H	3.22682967	-1.42803051	-0.75705883
F	1.10763193	-2.89640975	1.15735844
H	1.51967879	-2.12150204	0.75335157
F	-5.08554026	-0.09410499	-0.95475332
H	-4.16384356	0.02808317	-0.69932631
F	-2.21552207	2.64285657	0.12715147
H	-2.40600280	1.71471706	-0.02276562

1 5 1.0 6 1.5 24 1.0
2 6 2.0
3 8 2.0
4 5 1.0 11 1.0 12 1.0 25 1.0
5 8 1.0 10 1.0
6 7 1.0
7 13 1.0 14 1.0 15 1.0
8 19 1.5
9 16 1.0 17 1.0 18 1.0 19 1.0
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26 27 1.0
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28 29 1.0
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30 31 1.0
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32 33 1.0
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Ac-Ala-NMe2-beta-HFHFdonor

optimized M062X/junccpVTZ/H2O

0 1

N	-0.52613836	-1.05180671	0.11798384
O	-2.28498845	0.33138260	-0.11166287
O	1.91797778	-1.87731402	0.02974830
C	0.45491944	0.59810581	1.65223550
C	0.46896713	-0.00044316	0.24394657
C	-1.81351518	-0.83515568	-0.04291203
C	-2.73039144	-2.01147664	-0.14583934
C	1.82568694	-0.65246705	-0.03533264
C	4.19711904	-0.40937519	-0.44414430
H	0.24699783	0.75929592	-0.50079187
H	0.71745778	-0.17125720	2.37757717
H	1.16702289	1.41644011	1.73430822
H	-3.26978840	-1.94830958	-1.08968121

H	-3.46035481	-1.95224662	0.66029593
H	-2.19719918	-2.95512458	-0.08902864
H	4.53569548	-0.27965827	-1.47265379
H	4.17614537	-1.46404519	-0.19805724
H	4.88830976	0.11011420	0.21925803
N	2.86553716	0.15515311	-0.28454063
C	2.80969238	1.60272647	-0.41216076
H	3.31242737	1.89398254	-1.33409515
H	1.79159919	1.97161627	-0.44908024
H	3.32512260	2.07232533	0.42690363
H	-0.16316302	-1.99671105	0.15667894
H	-0.53712804	0.97974147	1.88398829
F	-4.74308147	0.53204773	-0.40675686
H	-3.78487521	0.45679306	-0.29234113
F	-1.23945995	2.60941545	-0.14709533
H	-1.61997312	1.72641409	-0.12215519

1 5 1.0 6 1.5 24 1.0
2 6 2.0
3 8 2.0
4 5 1.0 11 1.0 12 1.0 25 1.0
5 8 1.0 10 1.0
6 7 1.0
7 13 1.0 14 1.0 15 1.0
8 19 1.5
9 16 1.0 17 1.0 18 1.0 19 1.0
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20 21 1.0 22 1.0 23 1.0
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26 27 1.0
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28 29 1.0
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Ac-Ala-NMe2-beta

M062X/junccpVTZ/H2O optimized

0 1

N	-1.34374261	-0.43002951	0.09612889
O	-2.72157329	1.21913635	-0.58120851
O	0.89979006	-1.72415757	0.35757474
C	-0.09846630	1.25609204	1.38060170
C	-0.15826648	0.39842052	0.11333836
C	-2.55015373	0.04718942	-0.25431419
C	-3.68955043	-0.93893749	-0.22639445
C	1.04991239	-0.53855629	0.06407013
C	3.44072985	-0.83767520	-0.18713870
H	-0.19331606	1.03797150	-0.76646111
H	-0.06660426	0.60982859	2.25768346
H	0.78053500	1.89810425	1.38782807
H	-4.12748715	-0.99030868	-1.22178864
H	-4.45190336	-0.56573695	0.45529474
H	-3.38207432	-1.93369932	0.08521069

H	3.86121197	-0.95837204	-1.18636748
H	3.19015659	-1.80905976	0.22160910
H	4.18411732	-0.35308351	0.44655551
N	2.24597388	-0.01060665	-0.24623961
C	2.49588078	1.36929822	-0.62661352
H	3.10826705	1.38095218	-1.52827326
H	1.57869706	1.90654594	-0.83327019
H	3.03866786	1.88730056	0.16618107
H	-1.21302672	-1.39969984	0.34244578
H	-0.98911052	1.87889285	1.43190143

1 5 1.0 6 1.5 24 1.0
2 6 2.0
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4 5 1.0 11 1.0 12 1.0 25 1.0
5 8 1.0 10 1.0
6 7 1.0
7 13 1.0 14 1.0 15 1.0
8 19 1.5
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Ac-Ala-NMe2-beta-ureaacceptor

optimized M062X/junccpVTZ/H2O

0 1

N	-1.99662700	-0.86278900	-0.05668400
O	-4.23082800	-0.60233600	-0.17796000
O	0.51103300	-0.15780700	-0.24503300
C	-1.97675900	0.89355500	1.66748800
C	-1.73095200	0.53564700	0.19842900
C	-3.24531800	-1.33296900	-0.22927400
C	-3.36947000	-2.81025300	-0.49848400
C	-0.27139000	0.79927900	-0.15570000
C	1.56576100	2.28416300	-0.54127300
H	-2.39433100	1.11643200	-0.43981300
H	-1.30872500	0.31171700	2.30240700
H	-1.80256400	1.95199400	1.85349500
H	-3.81782000	-2.94422000	-1.48177900
H	-4.04569900	-3.24036700	0.23787800
H	-2.41589600	-3.33055500	-0.46352900
H	1.82825900	2.02542900	-1.56793500
H	2.16631400	1.68053000	0.13553300
H	1.77940000	3.33558000	-0.37213600
N	0.14509300	2.05780600	-0.29823700
C	-0.69838500	3.24424600	-0.29163900
H	-0.51445300	3.81564100	-1.20066500
H	-1.74958900	2.98705300	-0.25559000
H	-0.45674000	3.86726200	0.56970400
C	3.81364800	-1.13567800	0.13046000

N	3.28627800	-0.76718700	-1.06645500
H	3.77206500	-1.06537200	-1.89333700
H	2.31107100	-0.50782900	-1.12668100
N	3.03103300	-0.85230500	1.21215300
H	3.31100500	-1.26736800	2.08371800
H	2.05063400	-0.65639000	1.06820500
O	4.93300900	-1.63483900	0.23921600
H	-1.19523900	-1.47192500	-0.11929200
H	-3.00666200	0.65563700	1.92456100

1 5 1.0 6 1.5 32 1.0
2 6 2.0
3 8 2.0
4 5 1.0 11 1.0 12 1.0 33 1.0
5 8 1.0 10 1.0
6 7 1.0
7 13 1.0 14 1.0 15 1.0
8 19 1.5
9 16 1.0 17 1.0 18 1.0 19 1.0
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19 20 1.0
20 21 1.0 22 1.0 23 1.0
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24 25 1.5 28 1.5 31 2.0
25 26 1.0 27 1.0
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28 29 1.0 30 1.0
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Ac-Ala-NMe2-PPII-H2OH2OacceptorH2OH2O

optimized M062X/junccpVTZ/H2O

0 1

N	-0.36000000	-1.79700000	0.09300000
O	-1.12600000	-1.41900000	-1.98500000
O	-0.04500000	0.92900000	-0.00500000
C	-1.24200000	-0.98800000	2.20300000
C	-1.36900000	-0.95100000	0.68400000
C	-0.30100000	-1.94700000	-1.24400000
C	0.81600000	-2.80700000	-1.77100000
C	-1.18500000	0.49200000	0.20900000
C	-2.04000000	2.64600000	-0.34900000
H	-2.34600000	-1.31400000	0.37200000
H	-0.25600000	-0.62900000	2.50000000
H	-1.99600000	-0.35700000	2.67100000
H	1.32400000	-2.26900000	-2.56900000
H	0.38500000	-3.71300000	-2.19500000
H	1.53200000	-3.07400000	-0.99700000
H	-2.99800000	3.15000000	-0.41800000
H	-1.55600000	2.65800000	-1.32600000
H	-1.40200000	3.17500000	0.35700000

N	-2.25900000	1.27200000	0.09500000
C	-3.62300000	0.78600000	0.28400000
H	-3.94700000	0.17700000	-0.56100000
H	-3.71000000	0.20800000	1.20000000
H	-4.28300000	1.64400000	0.36900000
H	0.82000000	2.53200000	-0.38400000
H	1.54500000	0.09800000	-0.03900000
H	0.39000000	-2.15700000	0.67500000
H	-1.36800000	-2.00800000	2.56200000
O	2.45300000	-0.26000000	-0.05100000
O	1.40200000	3.28900000	-0.55700000
H	3.04000000	0.50400000	0.04800000
H	2.28700000	2.98100000	-0.32100000
O	4.01400000	2.14500000	0.13800000
H	4.71400000	2.26000000	-0.51300000
H	4.40600000	2.38200000	0.98400000
O	2.08900000	-2.34500000	1.65400000
H	2.41000000	-1.61200000	1.08900000
H	2.70800000	-3.07000000	1.53700000

1 5 1.0 6 1.5 26 1.0
2 6 2.0
3 8 2.0
4 5 1.0 11 1.0 12 1.0 27 1.0
5 8 1.0 10 1.0
6 7 1.0
7 13 1.0 14 1.0 15 1.0
8 19 1.5
9 16 1.0 17 1.0 18 1.0 19 1.0
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24 29 1.0
25 28 1.0
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28 30 1.0
29 31 1.0
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32 33 1.0 34 1.0
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35 36 1.0 37 1.0
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Ac-Ala-NMe2-PPII-HFdonor-HFHFacceptor

optimized M062X/junccpVTZ/H2O

0 1

N	-1.05244700	1.12627000	-0.83953500
O	-1.62538900	-0.97484200	-0.38079300
O	1.03082600	0.55365500	0.86269300

C	0.98521600	1.88621700	-1.94765600
C	0.21876300	0.69484200	-1.38550900
C	-1.90537400	0.23593400	-0.33347800
C	-3.17324300	0.73602000	0.28364900
C	1.04702200	0.03787100	-0.28562100
C	2.63548700	-1.57129000	0.49003900
H	0.01403500	-0.02784700	-2.16974500
H	1.17393300	2.61975800	-1.16392500
H	1.93921900	1.56015400	-2.35740800
H	-3.18146400	0.44529100	1.33349200
H	-4.01510400	0.24850600	-0.20512800
H	-3.27517200	1.81413300	0.20291200
H	3.36605400	-2.23293400	0.03932300
H	2.02604600	-2.13134000	1.19875800
H	3.15159900	-0.77375100	1.01804600
N	1.79956100	-1.00327200	-0.56861100
C	1.74357800	-1.68128700	-1.86744400
H	0.76781300	-2.14091500	-2.01712800
H	1.95513800	-0.98840000	-2.67831600
H	2.50093700	-2.45646400	-1.87613500
F	1.57875700	-0.26515900	3.17803900
H	1.39878400	-0.00084100	2.27525900
F	0.06323400	2.81690300	1.27094800
H	0.41929100	1.93164600	1.11384700
F	-3.26456800	-2.54474500	0.53297700
H	-2.60706900	-1.91581100	0.16752500
H	-1.21867100	2.11145300	-0.69969400
H	0.40583300	2.35303700	-2.74142300

1 5 1.0 6 1.5 30 1.0
2 6 2.0
3 8 2.0
4 5 1.0 11 1.0 12 1.0 31 1.0
5 8 1.0 10 1.0
6 7 1.0
7 13 1.0 14 1.0 15 1.0
8 19 2.0
9 16 1.0 17 1.0 18 1.0 19 1.0
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20 21 1.0 22 1.0 23 1.0
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24 25 1.0
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26 27 1.0
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28 29 1.0
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Ac-Ala-NMe2-PPII-HFHFacceptor

optimized M062X/junccpVTZ/H2O

0 1

N	1.65940400	-0.66428600	0.30743300

O	1.04918200	-0.81409900	-1.84203300
O	-0.53604800	1.02660700	0.43998700
C	0.33411200	-1.28780300	2.26062900
C	0.37515500	-1.16603900	0.74129800
C	1.88735000	-0.47934900	-1.01164300
C	3.20016500	0.14504600	-1.39369000
C	-0.72614400	-0.21129900	0.29317300
C	-2.95872300	0.23717400	-0.46273300
H	0.22180000	-2.13998600	0.28691600
H	0.49285400	-0.31441800	2.72449300
H	-0.63023300	-1.67646100	2.58280400
H	2.99604200	1.04955700	-1.96411000
H	3.73863900	-0.54539600	-2.04050500
H	3.81604800	0.39001600	-0.53254300
H	-3.89455700	-0.30973900	-0.41964800
H	-2.83411700	0.66770200	-1.45619900
H	-2.97752300	1.03635000	0.27236200
N	-1.86631500	-0.68689200	-0.15986400
C	-2.04976800	-2.10453300	-0.48538100
H	-1.29643900	-2.42786500	-1.20085900
H	-2.00431800	-2.72146800	0.40991600
H	-3.02922300	-2.22065300	-0.93545700
F	-1.46046300	3.01204600	-0.77780200
H	-1.14820000	2.22391400	-0.32621600
F	1.40177400	1.94188500	1.70609000
H	0.66262400	1.57300400	1.19939900
H	2.27153400	-0.24002500	0.98674700
H	1.11368600	-1.97091500	2.59176700

1 5 1.0 6 1.5 28 1.0
2 6 2.0
3 8 2.0
4 5 1.0 11 1.0 12 1.0 29 1.0
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6 7 1.0
7 13 1.0 14 1.0 15 1.0
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20 21 1.0 22 1.0 23 1.0
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24 25 1.0
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26 27 1.0
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Ac-Ala-NMe2-PPII-HFHFdonor-HFacceptor

M062X/junccpVTZ/H2O optimized

0 1

N	-0.97220523	-1.29001823	-0.96048975
O	-1.85309279	0.04039484	0.62105687

O	0.74713551	0.71433523	-1.17376159
C	1.07972645	-2.58194765	-0.97576465
C	0.30380320	-1.46112927	-0.29195585
C	-1.94885404	-0.53532527	-0.49016806
C	-3.18917335	-0.37750143	-1.30767099
C	1.10154544	-0.15084068	-0.35580237
C	2.97952554	1.19405698	0.26906603
H	0.10046544	-1.71857840	0.74492696
H	1.27481740	-2.32175896	-2.01625305
H	2.03330576	-2.74636305	-0.48082075
H	-3.29795237	0.67654760	-1.56100326
H	-4.04597658	-0.66552331	-0.70078665
H	-3.16468943	-0.97081992	-2.21624753
H	3.93110552	1.03099444	0.76586168
H	2.47517144	2.04686792	0.72441185
H	3.15532408	1.40673924	-0.78227645
N	2.17521557	-0.01558673	0.40994422
C	2.57566441	-0.92091575	1.47822709
H	2.65594627	-0.35427952	2.40449169
H	1.84946073	-1.70868881	1.62947745
H	3.54352370	-1.36292901	1.24260319
F	1.26643554	3.08267115	-1.59928283
H	1.10807945	2.14563197	-1.39470816
F	-3.83257792	1.35239574	1.38742255
H	-3.06432954	0.84871959	1.09322655
F	-0.12181734	0.11020473	2.43025943
H	-0.77413249	0.07550885	1.72632559
H	-1.07998290	-1.68158473	-1.88386756
H	0.50466094	-3.50491586	-0.94108476

1 5 1.0 6 1.5 30 1.0
2 6 2.0
3 8 2.0
4 5 1.0 11 1.0 12 1.0 31 1.0
5 8 1.0 10 1.0
6 7 1.0
7 13 1.0 14 1.0 15 1.0
8 19 2.0
9 16 1.0 17 1.0 18 1.0 19 1.0
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26 27 1.0
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28 29 1.0
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Ac-Ala-NMe2-PPII-HFHFdonor-HFHFacceptor

optimized M062X/junccpVTZ/H2O

0 1

N	0.94941700	-0.06663300	1.52128500
O	1.66730400	-0.95057200	-0.41438000
O	-0.70814400	1.23030800	-0.14140700
C	-1.13861300	-0.35375200	2.72317400
C	-0.40042100	-0.58449100	1.40779000
C	1.88260600	-0.24397200	0.59858800
C	3.20085600	0.43301900	0.77874800
C	-1.14039800	0.12325600	0.26935200
C	-2.96962000	0.33503600	-1.25306100
H	-0.33194900	-1.64729800	1.18834100
H	-1.19336600	0.71339900	2.93896600
H	-2.15128400	-0.74449300	2.66703800
H	3.30096400	1.18308200	-0.00554900
H	3.99361000	-0.30156600	0.65153600
H	3.28758100	0.91506500	1.74713000
H	-3.93125900	-0.14555700	-1.39904000
H	-2.41288100	0.32434800	-2.18932700
H	-3.12431800	1.36449500	-0.93918700
N	-2.24197000	-0.40237900	-0.22040800
C	-2.79782600	-1.70282600	0.13817800
H	-2.88921700	-2.30221000	-0.76524300
H	-2.16629700	-2.23342700	0.83802900
H	-3.78248300	-1.55881100	0.58049200
F	-1.07244700	2.69278300	-2.16268000
H	-0.99063400	2.09836600	-1.41779200
F	1.02019000	2.76142800	0.84820600
H	0.36341700	2.14878400	0.50662700
F	3.54693700	-1.15397800	-2.05414600
H	2.82010600	-1.07794900	-1.42729700
F	-0.19344100	-2.47266500	-1.13872100
H	0.51280800	-1.88889300	-0.85680700
H	1.15226800	0.56836100	2.27951600
H	-0.61313000	-0.85624800	3.53218300

1 5 1.0 6 1.5 32 1.0
2 6 2.0
3 8 2.0
4 5 1.0 11 1.0 12 1.0 33 1.0
5 8 1.0 10 1.0
6 7 1.0
7 13 1.0 14 1.0 15 1.0
8 19 2.0
9 16 1.0 17 1.0 18 1.0 19 1.0
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24 25 1.0
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26 27 1.0
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28 29 1.0
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30 31 1.0
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Ac-Ala-NMe2-PPII-HFHFdonor

optimized M062X/junccpVTZ/H2O

0 1

N	-0.80215400	1.52150800	-0.14562100
O	-1.74860300	-0.51240900	-0.27443100
O	0.69168800	0.31785900	1.70510400
C	1.36765800	2.30436600	-0.88531500
C	0.51745000	1.08119200	-0.56084400
C	-1.82937800	0.70879800	0.00986700
C	-3.11700900	1.26811900	0.52243700
C	1.16612500	0.26631500	0.57553600
C	2.96088800	-1.14170200	1.34804500
H	0.39078200	0.46019700	-1.44492100
H	1.47329800	2.92981200	0.00184900
H	2.36045400	2.00499000	-1.21127200
H	-3.37410400	0.74645900	1.44336300
H	-3.89928500	1.06351000	-0.20705200
H	-3.06006500	2.33575100	0.70952600
H	2.62034600	-2.17897000	1.38384700
H	2.75871000	-0.66625300	2.30131300
H	4.03153600	-1.13078200	1.15192400
N	2.28449300	-0.41751400	0.28385300
C	2.80805900	-0.67050800	-1.04758000
H	2.86840000	-1.74744700	-1.20700300
H	2.17301100	-0.25631900	-1.82009900
H	3.80747300	-0.24360100	-1.14288600
F	-3.80542300	-1.87673900	0.04965100
H	-3.00467300	-1.35060100	-0.07723600
F	0.06195000	-2.01086300	-1.13317100
H	-0.61122700	-1.41291500	-0.79720500
H	-0.90725900	2.47722800	0.15876400
H	0.90004600	2.88632600	-1.67712900

1 5 1.0 6 2.0 28 1.0
2 6 2.0
3 8 2.0
4 5 1.0 11 1.0 12 1.0 29 1.0
5 8 1.0 10 1.0
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26 27 1.0
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Ac-Ala-NMe2-PPII-HFtrans

optimized M062X/junccpVTZ/H2O

0 1

N	1.78855100	-0.39699400	0.56471400
O	1.78547200	0.08913500	-1.62679100
O	-0.49991000	1.02684900	0.51868600
C	0.25452500	-1.81785900	1.80053900
C	0.54246100	-1.11955200	0.47614700
C	2.30948400	0.20627700	-0.52474100
C	3.55953500	1.01678100	-0.31442100
C	-0.60242900	-0.15594900	0.14904800
C	-2.76147100	0.33042200	-0.76573800
H	0.64569700	-1.84327400	-0.32877500
H	0.15849800	-1.07959700	2.59723400
H	-0.67247700	-2.38525600	1.74815700
H	3.33074200	2.06072600	-0.52473400
H	4.31106900	0.68786600	-1.02920400
H	3.95443200	0.93167400	0.69447800
H	-3.46349300	-0.15114300	-1.43951800
H	-2.36275700	1.22364300	-1.24105900
H	-3.27942500	0.62020900	0.14838100
N	-1.68320700	-0.60985000	-0.47573000
C	-1.92703100	-1.99420500	-0.85926800
H	-2.00328900	-2.06881200	-1.94349700
H	-1.14059100	-2.65249400	-0.51381300
H	-2.86631400	-2.32438100	-0.41692800
F	-1.96516700	2.97954800	0.73207900
H	-1.42880600	2.17260100	0.61398000
H	2.16315600	-0.18440700	1.47473900
H	1.06770700	-2.49873600	2.04441300

1 5 1.0 6 1.5 26 1.0
2 6 2.0
3 8 2.0
4 5 1.0 11 1.0 12 1.0 27 1.0
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7 13 1.0 14 1.0 15 1.0
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Ac-Ala-NMe2-PPII

optimized M062X/junccpVTZ/H2O

0 1

N	1.53182300	0.71494800	-0.07939000
O	1.48676000	-1.24566400	1.01433300

O	-0.41806800	-0.44863900	-1.61445400
C	-0.20807900	2.40378000	-0.22935600
C	0.14437800	0.98993000	0.21576600
C	2.09889100	-0.44194200	0.31820900
C	3.51302400	-0.69099900	-0.13342500
C	-0.75844300	-0.01298600	-0.51944400
C	-2.82715900	-1.27815000	-0.55950700
H	0.01367300	0.88532500	1.29016700
H	-0.06209900	2.50210300	-1.30558300
H	-1.24901800	2.63040200	-0.00576500
H	3.50661200	-1.52591200	-0.83329300
H	4.10915000	-0.98102700	0.72904900
H	3.96186700	0.17451600	-0.61366900
H	-2.88850700	-2.18541100	0.04414000
H	-2.45077800	-1.52680300	-1.54472800
H	-3.82473900	-0.84849600	-0.64672400
N	-1.93137000	-0.31923800	0.06733700
C	-2.30309100	0.12115300	1.40590500
H	-1.76953000	-0.43910600	2.17604100
H	-2.12181000	1.18388300	1.54448800
H	-3.36882000	-0.05064200	1.53181300
H	2.01011800	1.29279300	-0.75087400
H	0.42405000	3.12811200	0.28138000

1 5 1.0 6 1.5 24 1.0
2 6 2.0
3 8 2.0
4 5 1.0 11 1.0 12 1.0 25 1.0
5 8 1.0 10 1.0
6 7 1.0
7 13 1.0 14 1.0 15 1.0
8 19 1.5
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Ac-Ala-NMe2-PPII-ureaacceptor

optimized M062X/junccpVTZ/H2O

0 1 0 1 0 1

N(Fragment=1)	-0.13772400	1.47991200	0.40911700
O(Fragment=1)	-0.04007600	1.18862100	-1.81357100
O(Fragment=1)	0.51256700	-1.17844800	0.45461700
C(Fragment=1)	1.64290700	1.31812200	2.05156400
C(Fragment=1)	1.24246000	1.09893000	0.59705400
C(Fragment=1)	-0.69276900	1.49295000	-0.82054300
C(Fragment=1)	-2.12688100	1.94418600	-0.89564600
C(Fragment=1)	1.43208500	-0.38154400	0.24282000
C(Fragment=1)	2.86125500	-2.14383900	-0.60737500
H(Fragment=1)	1.84830800	1.71469900	-0.06377600
H(Fragment=1)	1.02590100	0.69880900	2.70369500
H(Fragment=1)	2.68500600	1.04820000	2.21080000

H(Fragment=1)	-2.61932400	1.43104700	-1.71674700
H(Fragment=1)	-2.14109300	3.01583500	-1.09675500
H(Fragment=1)	-2.66560600	1.75776600	0.03190900
H(Fragment=1)	3.05160900	-2.20776000	-1.67943800
H(Fragment=1)	1.99113700	-2.73836300	-0.35715400
H(Fragment=1)	3.73184800	-2.52385100	-0.07384400
N(Fragment=1)	2.62471400	-0.75705900	-0.23259100
C(Fragment=1)	3.70366100	0.17354400	-0.54465900
H(Fragment=1)	3.54010600	0.66212100	-1.50648700
H(Fragment=1)	3.82209200	0.92655900	0.22890700
H(Fragment=1)	4.62920400	-0.39364900	-0.59734800
C(Fragment=2)	-2.92487000	-1.03619000	0.23672500
N(Fragment=2)	-2.14084700	-1.39224700	-0.81910700
H(Fragment=2)	-2.54902500	-1.29882400	-1.73280100
H(Fragment=2)	-1.13496700	-1.33388000	-0.72890300
N(Fragment=2)	-2.27066800	-0.94687600	1.42536100
H(Fragment=2)	-2.78347400	-0.57805500	2.20618900
H(Fragment=2)	-1.25897700	-0.93076700	1.43477800
O(Fragment=1)	-4.13768000	-0.85352700	0.12871000
H(Fragment=1)	-0.71458800	1.65032900	1.21670500
H(Fragment=1)	1.50793600	2.36355500	2.32312100

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Coordinates of structures of Ac-Pro_2-NMe_2 in a PPII conformation as a function of ring pucker and explicit solvation

Ac-Pro2-NMe2-trans-nn-4HF

M062X/6311pp2d2p/H2O optimized

0 1

C	-4.68874034	0.33955575	-0.89860260
C	-3.45905197	0.30188707	-0.04240630
O	-3.03113259	1.30588020	0.56477785
H	-5.36060914	-0.47751878	-0.64176940
N	-2.80089581	-0.84996188	0.05580188
C	-1.59507189	-0.95043371	0.86663137
C	-0.48043791	-0.09427131	0.27944079
O	-0.42854716	0.20481407	-0.92399870
C	-1.25386063	-2.45079543	0.80439575
C	-1.81461804	-2.87600131	-0.55531213
C	-3.12432071	-2.10000013	-0.64942231
H	-3.41873812	-1.88664025	-1.67251447
H	-1.80095810	-0.61022639	1.87910520
H	-1.78449985	-2.95885057	1.60874017
H	-1.96583939	-3.94899031	-0.63095679
H	-3.93410483	-2.61688189	-0.13258499
H	-0.18923584	-2.63569895	0.91907912
H	-1.14593541	-2.55984629	-1.35658170
N	0.48068065	0.31050769	1.10690826
C	1.49421338	1.24442256	0.62906172
C	2.44711461	0.57709629	-0.35264015
O	2.64370050	-0.66412368	-0.29553330
C	2.21029037	1.68753955	1.92104501
C	1.99297359	0.51073434	2.87597674
C	0.57532285	0.04990812	2.55412952
H	0.41911103	-1.00524395	2.76067521
H	0.99581827	2.06735742	0.12378355
H	1.72209817	2.58407546	2.29959491
H	2.10209464	0.79539477	3.91839375
H	-0.16794527	0.64612039	3.08558153
H	3.26148493	1.91159847	1.75590084
H	2.69650942	-0.29193176	2.65839691
N	3.06614929	1.33036908	-1.23910128
C	3.92200185	0.70664614	-2.24812973
H	4.91368678	0.51147335	-1.84234838
H	4.00221748	1.38837551	-3.08886268
H	3.47850516	-0.22548865	-2.58464687
C	2.96090634	2.78956330	-1.28119644
H	2.18025352	3.09653270	-1.97599013
H	3.91536340	3.18157614	-1.62044948
H	2.76405321	3.20009150	-0.29741173
F	4.54651669	-2.12769686	-1.06955948
H	3.84604750	-1.53157133	-0.81733649
F	1.98202518	-2.36969264	1.37357912
H	2.17020116	-1.65957748	0.75013543
H	-4.39182702	0.22093449	-1.94083990
H	-5.19291330	1.29136785	-0.76803267
F	-2.02034316	-0.18685099	-2.74364305
H	-1.41876956	-0.06031456	-1.98889497
F	-4.25786895	3.38583068	0.38450725
H	-3.76307049	2.53549507	0.45082314

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Ac-Pro2-NMe2-trans-nn-5HF

M062X/6311pp2d2p/H2O optimized

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C	-4.69348659	0.38650585	-0.91438406
C	-3.46548019	0.44339234	-0.05723307
O	-2.98853245	1.51474464	0.36799056
H	-5.40492614	-0.33556706	-0.51722542
N	-2.85791615	-0.70389279	0.24123681
C	-1.67324002	-0.71567542	1.08681684
C	-0.50694782	-0.02154958	0.39890030
O	-0.45717257	0.06315460	-0.85003943
C	-1.40083561	-2.21938908	1.29454254
C	-1.99037988	-2.85789365	0.03396130
C	-3.25927431	-2.04752438	-0.20391270
H	-3.56146850	-2.02463520	-1.24646512
H	-1.88085691	-0.19822222	2.02056196
H	-1.94826615	-2.54687628	2.17732134
H	-2.19430227	-3.91748162	0.15763297
H	-4.08596320	-2.40782142	0.41003268

H	-0.34585146	-2.43266671	1.44309321
H	-1.31032450	-2.72987821	-0.80897914
N	0.45917183	0.45392971	1.16526617
C	1.58053096	1.21029157	0.60766461
C	2.55592933	0.29360164	-0.13059949
O	2.42990906	-0.95539462	-0.03793538
C	2.21263210	1.86700453	1.84888609
C	1.90075101	0.87103398	2.96644632
C	0.48400910	0.41250243	2.64403783
H	0.27655536	-0.59303182	2.99823906
H	1.19362963	1.94205080	-0.09819097
H	1.71757986	2.81925480	2.03191557
H	1.96707282	1.31667012	3.95437445
H	-0.25827062	1.10841725	3.03549435
H	3.27650735	2.04696826	1.72122779
H	2.58141174	0.02142386	2.92154960
N	3.52482097	0.83351191	-0.83795595
C	4.45049526	-0.03694655	-1.56097410
H	4.71630114	-0.89045744	-0.94529240
H	5.34299378	0.53559568	-1.79260304
H	3.99202129	-0.38470571	-2.48644253
C	3.64998849	2.25799030	-1.13051997
H	3.44163141	2.42048032	-2.18667401
H	4.66767758	2.57026216	-0.90697675
H	2.96786589	2.85309928	-0.53778952
F	2.78957265	-2.72898735	-1.80205066
H	2.68708069	-2.03824412	-1.15456664
F	1.82227602	-2.23658787	2.00329195
H	2.02238019	-1.71351604	1.22190209
H	-4.40723294	0.06587296	-1.91631412
H	-5.14847171	1.37028375	-0.96210473
F	-2.07355137	-0.65522426	-2.63319792
H	-1.50741854	-0.41171193	-1.90223456
F	-4.13006237	3.59077304	-0.16127851
H	-3.67070140	2.74658474	0.04658166
F	1.09483478	1.13552552	-2.51092717
H	0.52139846	0.73341729	-1.86235694

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Ac-Pro2-NMe2-trans-nn-6HF

M062X/6311pp2d2p/H2O optimized

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C	4.69938648	0.20035165	-1.03940956
C	3.49403652	-0.09866311	-0.20519029
O	3.18578065	-1.28658539	0.07490780
H	5.32305750	0.94918966	-0.55466323
N	2.76075355	0.91650034	0.22208803
C	1.60595203	0.74919360	1.10053061
C	0.43035168	0.12058750	0.36467983
O	0.41663073	0.05688711	-0.88589157
C	1.29255862	2.19257401	1.54346564
C	1.75113551	3.02335818	0.34413328
C	3.04147972	2.33519554	-0.07893336
H	3.26727523	2.45489316	-1.13396410
H	1.86921038	0.10567115	1.93936321
H	1.89433994	2.42319829	2.42122101
H	1.90776610	4.06869429	0.59245602
H	3.88905092	2.66982935	0.51975149
H	0.24345087	2.33155904	1.78735922
H	1.01752066	2.96326741	-0.46111613
N	-0.56274877	-0.34396411	1.10005003
C	-1.61866092	-1.16387129	0.50510463
C	-2.66607594	-0.30319664	-0.19756240
O	-2.64554702	0.94635749	-0.05102680
C	-2.19723321	-1.92650609	1.71230918
C	-1.94833643	-0.97061767	2.87879755
C	-0.56296059	-0.41737776	2.57648418
H	-0.39382534	0.56459982	3.00707473
H	-1.16540515	-1.83310239	-0.22343063
H	-1.63152151	-2.84741429	1.84491521
H	-1.98467663	-1.46783593	3.84339089
H	0.21632608	-1.11123829	2.89305913
H	-3.24610338	-2.17542163	1.57689087
H	-2.67861502	-0.16145023	2.87407736
N	-3.58949968	-0.89343277	-0.92679252
C	-4.58517233	-0.07188038	-1.61216322
H	-4.94159777	0.70981535	-0.94829784
H	-5.41457723	-0.71103971	-1.89702481
H	-4.15095784	0.37916092	-2.50422565

C	-3.57748397	-2.30572053	-1.29610208
H	-3.31129739	-2.39349575	-2.34850181
H	-4.57138870	-2.71602236	-1.13413948
H	-2.87088114	-2.87077185	-0.70232460
F	-3.35562556	2.82750874	-1.58164888
H	-3.11928644	2.08740844	-1.03076265
F	-1.97571672	2.19886478	1.99085849
H	-2.18821143	1.68453497	1.20642937
H	4.37189465	0.59853351	-1.99983634
H	5.26702870	-0.71013619	-1.19758627
F	1.97301326	0.99587870	-2.62967545
H	1.42395255	0.66583243	-1.92215911
F	4.64896277	-3.12135475	-0.75205255
H	4.08505712	-2.40787509	-0.43638154
F	-1.16116174	-0.87982715	-2.61469491
H	-0.58242166	-0.52977411	-1.94353193
F	1.27166470	-2.50721192	1.11538301
H	1.99629197	-2.01289558	0.73023216

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Ac-Pro2-NMe2-trans-nn-HF212

M062X/6311pp2d2p/H2O optimized

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C	4.65429875	0.35321610	-1.10342763
C	3.46665138	0.03464633	-0.25152047
O	3.23919605	-1.15008701	0.11391237
H	5.20466087	1.19814638	-0.69442806
N	2.66582871	1.02445183	0.10137898
C	1.50608381	0.84164649	0.97047312
C	0.37693599	0.12419340	0.23883046
O	0.35823195	-0.01300895	-0.99369851
C	1.11681129	2.28730767	1.33189316
C	1.51638791	3.06610740	0.07733332
C	2.84115710	2.42838614	-0.32141579
H	3.03613208	2.47206781	-1.38883076
H	1.78449169	0.25204213	1.84337271
H	1.71307066	2.60423831	2.18643496
H	1.61548651	4.13232121	0.25762165
H	3.67648921	2.86848596	0.22391840
H	0.06324833	2.38190358	1.57812142
H	0.77856347	2.91423545	-0.71122483
N	-0.61506029	-0.35180388	0.98595060
C	-1.58179164	-1.25874597	0.37704347
C	-2.59912720	-0.49866515	-0.46220578
O	-2.80468949	0.72264348	-0.24349246
C	-2.23216629	-1.95991737	1.58700942
C	-2.04964548	-0.95183943	2.72419936
C	-0.66302458	-0.37922799	2.45746153
H	-0.53231629	0.61920411	2.86440793
H	-1.04145060	-1.95029728	-0.26435770
H	-1.67903068	-2.87422049	1.79592375
H	-2.12089752	-1.41115852	3.70577744
H	0.11819355	-1.04337161	2.83021895
H	-3.27299474	-2.21735061	1.40593177
H	-2.79427202	-0.15949247	2.65355393
N	-3.26796798	-1.14469414	-1.39651012
C	-4.21794265	-0.40428737	-2.22644365
H	-5.10172824	-0.13695887	-1.64926900
H	-4.50674756	-1.03771230	-3.05840287
H	-3.75234063	0.50001280	-2.60926290
C	-3.15750417	-2.57825591	-1.65883789
H	-2.62399912	-2.74482644	-2.59318291
H	-4.16187660	-2.98640302	-1.74303524
H	-2.65154111	-3.09379222	-0.85237432
F	-4.47935107	2.45284549	-0.99307821
H	-3.87533221	1.75311923	-0.75885542
F	-2.15440677	2.15794890	1.67867514
H	-2.33203516	1.55354616	0.95109617
H	4.30356905	0.62322714	-2.09967807
H	5.30070416	-0.51549949	-1.16680379
F	1.90364732	0.74402269	-2.74476798
H	1.31960586	0.46618542	-2.02032686
F	4.86068899	-2.92056574	-0.50997395
H	4.23250878	-2.22778282	-0.27324265
F	1.37408164	-2.41671480	1.18169974
H	2.07364083	-1.89714142	0.78204047

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Ac-Pro2-NMe2-trans-nn-HF221

M062X/6311pp2d2p/H2O optimized

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C	4.59441785	-0.49558081	-0.76687700
C	3.32570805	-0.31830306	0.00564119
O	2.88313570	-1.24244300	0.73741519
H	5.26621985	0.34404963	-0.59832497
N	2.67842967	0.82989704	-0.10721575
C	1.47435609	1.13695328	0.65919679
C	0.27346274	0.34667888	0.15650365
O	0.30195218	-0.21778220	-0.96252441

C	1.29228796	2.65039755	0.43002382
C	1.88138942	2.85549515	-0.96641599
C	3.11060866	1.95555392	-0.96003792
H	3.38412736	1.59277150	-1.94621977
H	1.63348371	0.89137728	1.70825386
H	1.87860571	3.18536112	1.17554468
H	2.13424762	3.89216853	-1.16771809
H	3.96584122	2.45011304	-0.49876650
H	0.25291051	2.95640634	0.50844582
H	1.17725471	2.51566266	-1.72703760
N	-0.78080424	0.28953614	0.94611135
C	-1.89115458	-0.62481312	0.66922727
C	-2.85717238	-0.04159197	-0.36358139
O	-2.78472362	1.15308340	-0.70217558
C	-2.55522773	-0.79062678	2.04985511
C	-2.26843266	0.54644021	2.73362188
C	-0.83438997	0.83750983	2.31749487
H	-0.59774857	1.89690359	2.31495894
H	-1.47928646	-1.55926526	0.29224989
H	-2.06116686	-1.60405893	2.57934599
H	-2.37616321	0.49859897	3.81310816
H	-0.12735771	0.29103289	2.94266144
H	-3.61617745	-1.01131461	1.97288696
H	-2.92938603	1.32260859	2.34809959
N	-3.78871320	-0.85086115	-0.85723568
C	-4.67755044	-0.36399267	-1.90542180
H	-4.75074454	0.71513886	-1.85148881
H	-5.65954163	-0.80873362	-1.76456779
H	-4.28934048	-0.65617386	-2.88247019
C	-3.81207338	-2.29482984	-0.65181540
H	-3.28347133	-2.79387902	-1.46373032
H	-4.84965261	-2.61926261	-0.64323118
H	-3.36692758	-2.57499742	0.29547369
F	-1.95005899	3.04963979	0.57042095
H	-2.23967453	2.25643288	0.07532955
H	4.35270068	-0.53269049	-1.82911374
H	5.07605397	-1.42080742	-0.46968725
F	2.05984133	-0.31968055	-2.75805180
H	1.43339465	-0.24079242	-2.04076615
F	4.23233997	-3.31473760	0.97990455
H	3.71270255	-2.50975642	0.87852400
F	-1.31682626	-1.52898897	-2.36713564
H	-0.73683302	-1.02472999	-1.80235668
F	0.77749547	-1.85173379	1.95212933
H	1.56812840	-1.58126692	1.48735847

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Ac-Pro2-NMe2-trans-nn-HF3

M062X/6311pp2d2p/H2O optimized

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C	-4.81280420	1.49407933	0.09294188
C	-3.58269251	0.84447534	0.66809841
O	-3.03971201	1.24294103	1.69701955
H	-5.58298328	0.75363062	-0.11924322
N	-3.08539464	-0.20976461	-0.01133292
C	-1.90677602	-0.90104542	0.47520828
C	-0.67582873	-0.00819831	0.39462182
O	-0.58765690	0.94719506	-0.39306455
C	-1.78889052	-2.10799860	-0.47537341
C	-2.40126755	-1.57878845	-1.77467896
C	-3.58268332	-0.74642157	-1.28451124
H	-3.83890193	0.06241353	-1.96311871
H	-2.04643994	-1.20130162	1.51200952
H	-2.39496886	-2.92063057	-0.07601733
H	-2.70526180	-2.37191956	-2.45212630
H	-4.46317513	-1.36926276	-1.11334553
H	-0.76535558	-2.45737325	-0.58142034
H	-1.68924517	-0.93284718	-2.28982035
N	0.35175144	-0.30720828	1.18918076
C	1.50387785	0.58442966	1.24417990
C	2.31144444	0.52681759	-0.04591668
O	2.27310774	-0.50143555	-0.76883421
C	2.30150005	0.06623157	2.45790710
C	1.89849459	-1.40799585	2.55135292
C	0.41957877	-1.39580193	2.17886442
H	0.09016119	-2.33261704	1.73780608
H	1.14864668	1.60202264	1.38202414
H	1.97745686	0.60943278	3.34399707
H	2.06641757	-1.82405624	3.54051731

H	-0.20551596	-1.15239680	3.03932625
H	3.37318855	0.20788473	2.34014482
H	2.45331112	-2.00036181	1.82517465
N	3.05463376	1.56484398	-0.37487666
C	3.76483722	1.55792904	-1.65356272
H	4.65640750	0.93524716	-1.59643921
H	4.04995924	2.57854115	-1.88703277
H	3.11220172	1.18211165	-2.43640457
C	3.23015335	2.74909998	0.46534127
H	2.57887734	3.55401339	0.12769606
H	4.26560102	3.06798200	0.38208763
H	3.03296750	2.52765534	1.50744088
F	3.66978120	-1.39911419	-2.66695933
H	3.17512189	-0.99751858	-1.95751577
F	1.43843924	-2.79456232	-0.33051162
H	1.70333948	-1.87560198	-0.44260547
H	-4.55080352	1.98759963	-0.84298158
H	-5.18784199	2.22618726	0.80027300
F	-2.23199138	1.94211948	-1.90930330
H	-1.62573123	1.49960250	-1.28806041

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Ac-Pro2-NMe2-trans-nn

M062X/6311pp2d2p/H2O optimized

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C	-4.61988885	-0.32445362	-1.70233814
C	-3.43347815	0.37396680	-1.08733222
O	-2.92995911	1.37821962	-1.59003509
H	-5.39282026	-0.51834807	-0.96001426
N	-2.94489779	-0.15890208	0.04797847
C	-1.77884076	0.42094164	0.68818727
C	-0.52036475	0.17654111	-0.14296589
O	-0.43624768	-0.76670591	-0.92252618
C	-1.68517433	-0.35367905	2.01485229
C	-2.25521466	-1.72728544	1.64966438
C	-3.40115467	-1.39418266	0.69487568
H	-3.57196423	-2.17792719	-0.03990640
H	-1.92590923	1.48870926	0.83414029
H	-2.30953570	0.13646368	2.76117682
H	-2.59162386	-2.28937555	2.51670046
H	-4.33180621	-1.21449399	1.23713957
H	-0.66442255	-0.40464558	2.38847580
H	-1.49980146	-2.31056604	1.12484541
N	0.50391544	1.01833817	0.07699155
C	1.79621161	0.74989354	-0.52773592
C	2.42765608	-0.49135441	0.12347896
O	2.03680515	-0.87697906	1.22044545
C	2.59781504	2.01915645	-0.19762293
C	2.03945213	2.42670121	1.16801552
C	0.54609799	2.11522943	1.05475638
H	0.11927077	1.81149795	2.00854369
H	1.67058672	0.59045084	-1.59498664
H	2.38160539	2.78166956	-0.94546833
H	2.22214643	3.47137468	1.40436884
H	-0.01200522	2.97395897	0.67777799
H	3.67104640	1.84404774	-0.18166123
H	2.48407580	1.81058792	1.94796597
N	3.43913026	-1.08025987	-0.54744497
C	4.05429056	-2.29018395	-0.02607090
H	5.11894848	-2.12532526	0.14057310
H	3.93570856	-3.10120428	-0.74589213
H	3.57722295	-2.56087724	0.90803702
C	3.89735891	-0.67270600	-1.86796089
H	3.37771500	-1.22359270	-2.65414298
H	4.96167788	-0.88804627	-1.94041995
H	3.76548235	0.39172476	-2.02908377
H	-4.30806086	-1.28388958	-2.11655150
H	-5.01795617	0.29578551	-2.49818818

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Ac-Pro2-NMe2-trans-nn-P2HFHF

M062X/6311pp2d2p/H2O optimized

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C	4.82267444	-1.27375798	-1.37409855
C	3.69766664	-1.10988774	-0.38417702
O	3.23926714	-2.05792233	0.25241076
H	5.59470117	-0.52012194	-1.22645572
N	3.20891770	0.13505402	-0.22967627
C	2.09170498	0.37508931	0.66434947
C	0.81649458	-0.25245266	0.10003861
O	0.67879605	-0.49676764	-1.09207053
C	1.99742894	1.90896702	0.69916367
C	2.46292705	2.30816925	-0.70407771
C	3.59936137	1.32697826	-0.99190808
H	3.69540490	1.09751163	-2.05094457
H	2.29720362	-0.05394834	1.64300007
H	2.69243543	2.28472229	1.44994427
H	2.78979823	3.34285195	-0.76254495
H	4.55491895	1.71015208	-0.62858370
H	0.99717411	2.25879032	0.94152661
H	1.65701491	2.15674764	-1.42113517
N	-0.17295603	-0.49626940	0.98470256
C	-1.34603763	-1.23113064	0.54384067
C	-2.22443663	-0.38794009	-0.36972770
O	-2.20273934	0.86709849	-0.28770950
C	-2.06457830	-1.59350458	1.86045358
C	-1.59569913	-0.50874375	2.83457435
C	-0.13921702	-0.28630416	2.43841198
H	0.20710283	0.71686529	2.67377246
H	-1.02680208	-2.11068023	-0.00996216
H	-1.72003040	-2.57363307	2.18656980
H	-1.69891552	-0.80823983	3.87370758
H	0.51686628	-1.01935561	2.91237089
H	-3.14588721	-1.62917432	1.74835834
H	-2.15890819	0.41066812	2.67871609

N	-3.01861455	-1.00082161	-1.22638485
C	-3.81016946	-0.20001775	-2.15996845
H	-4.64652979	0.27303163	-1.64765722
H	-4.18619530	-0.85639111	-2.93724824
H	-3.18629971	0.56761112	-2.61009539
C	-3.15044142	-2.45592703	-1.30980022
H	-2.46121274	-2.86269350	-2.04880533
H	-4.16944751	-2.68309164	-1.60836342
H	-2.97446333	-2.92171354	-0.34668455
F	-3.62568324	2.74887931	-1.15453125
H	-3.12118074	1.98960780	-0.86889652
F	-1.20311557	2.38926349	1.39643509
H	-1.52072070	1.73118558	0.76864146
H	4.43638493	-1.16017070	-2.38774084
H	5.24668606	-2.26605085	-1.26260803

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Ac-Pro2-NMe2-trans-nx-4HF

M062X/6311pp2d2p/H2O optimized

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C	4.46773974	-0.56592381	0.64054497
C	3.27935259	0.22591227	0.18463630
O	2.97340510	1.32725266	0.68728654
H	5.06429026	-0.88852449	-0.21103006
N	2.52629810	-0.28287508	-0.78692061
C	1.35826323	0.43103243	-1.27904591
C	0.25072577	0.45222741	-0.23584638
O	0.22561440	-0.32626256	0.73247629
C	0.92763019	-0.40331051	-2.50048214
C	1.36070431	-1.81879175	-2.10954762
C	2.71026308	-1.59292055	-1.43324415
H	2.94362099	-2.34888277	-0.68902707
H	1.62660323	1.45180594	-1.53994832
H	1.48464419	-0.06021604	-3.37130547
H	1.43591949	-2.48742477	-2.96228064
H	3.51898497	-1.53253209	-2.16296906
H	-0.13599731	-0.31411418	-2.70907637
H	0.65554216	-2.24331535	-1.39350202
N	-0.75946282	1.29378756	-0.43373453
C	-1.90737580	1.27051823	0.47493531
C	-2.43286814	-0.14461396	0.63212324
O	-2.53352083	-0.86759192	-0.39848098
C	-2.92603092	2.18413590	-0.22256159
C	-2.03381651	3.19241925	-0.94829347
C	-0.87493029	2.34083027	-1.46540030
H	-1.10832410	1.88597349	-2.42688101
H	-1.60664336	1.68142758	1.43476127
H	-3.60820941	2.63936404	0.48971897
H	-1.66038645	3.93565825	-0.24464077
H	0.05017245	2.90540552	-1.54105438
H	-3.50263367	1.60598836	-0.94431473
H	-2.55090712	3.70529659	-1.75413215
N	-2.82092853	-0.56938985	1.81470266
C	-3.42228139	-1.89459565	1.96335210
H	-4.23088860	-1.82377643	2.68522359
H	-2.67629300	-2.60305504	2.32158420
H	-3.81382928	-2.22954178	1.01017322
C	-2.56919010	0.18200766	3.04966964
H	-1.50350032	0.36049599	3.17410429
H	-2.91880759	-0.42161661	3.87981233
H	-3.11182850	1.12404174	3.05300411
F	-1.51086258	-3.16728342	-0.29185131
H	-1.91291129	-2.30229333	-0.33474951
F	-2.49208102	-0.03512524	-2.71984852
H	-2.48836095	-0.33788556	-1.80005155
H	4.11388563	-1.45349028	1.16548588
H	5.07161665	0.03869513	1.30931736
F	1.73314659	-2.12939060	1.42751369
H	1.16913637	-1.40504948	1.10697855
F	4.36104082	2.21619867	2.46007353
H	3.79945926	1.84656394	1.73818548

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Ac-Pro2-NMe2-trans-nx-5HF

M062X/6311pp2d2p/H2O optimized

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C	-4.48013984	0.43746848	-0.71502448
C	-3.25989754	0.37339613	0.15259948
O	-2.80979383	1.36799860	0.75751540
H	-5.17676388	-0.35815175	-0.45668296
N	-2.62987391	-0.79464669	0.26217354
C	-1.43895839	-0.91590086	1.08840588
C	-0.29935728	-0.08160076	0.53009106
O	-0.27294967	0.25389537	-0.68050878
C	-1.10433007	-2.41995437	1.01776148
C	-1.67893651	-2.84002057	-0.33798352
C	-2.98036619	-2.04913511	-0.42302465
H	-3.28749690	-1.84470933	-1.44393322
H	-1.65338130	-0.58803526	2.10193840
H	-1.62489001	-2.92760884	1.82825965
H	-1.84487325	-3.91134127	-0.40691912
H	-3.78938399	-2.54789532	0.11240373
H	-0.03829273	-2.60935657	1.12098306
H	-1.00983696	-2.53686803	-1.14418573
N	0.70421827	0.21420237	1.33445313
C	1.91532620	0.88025173	0.83500302
C	2.46981959	0.15741462	-0.38318704
O	2.32326395	-1.09349003	-0.46579252
C	2.88255540	0.79186639	2.02814141

C	1.94516677	0.81465259	3.23442068
C	0.76770195	-0.04656000	2.78873515
H	0.95285347	-1.10631187	2.95626531
H	1.67459943	1.91308955	0.59058061
H	3.60161664	1.60573652	2.02282897
H	1.60724842	1.83188706	3.42782295
H	-0.16224285	0.24748901	3.26553796
H	3.42150989	-0.15491962	1.98862825
H	2.41213366	0.42509159	4.13402956
N	3.12793947	0.84887275	-1.28650005
C	3.67420204	0.20412176	-2.47977777
H	4.75221372	0.34901121	-2.49863508
H	3.23413059	0.66984076	-3.35979391
H	3.44652950	-0.85360511	-2.47110267
C	3.36252156	2.29437408	-1.18848059
H	2.49257196	2.84432607	-1.53883427
H	4.21811486	2.52827877	-1.81395138
H	3.60425610	2.58078059	-0.16997525
F	1.08788355	-2.14399918	-2.40986012
H	1.53950309	-1.74196708	-1.67584806
F	2.28246058	-2.50931478	1.56320664
H	2.28216171	-1.95406228	0.77326685
H	-4.17966760	0.30133040	-1.75426201
H	-4.95852792	1.40408974	-0.59674922
F	-1.82923934	-0.27039862	-2.58290783
H	-1.26078222	-0.12828238	-1.82709863
F	-3.97356145	3.48619481	0.54907415
H	-3.50536591	2.62431509	0.62721301
F	0.23322694	2.60621120	-1.40900720
H	0.05313356	1.71113239	-1.13301747

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Ac-Pro2-NMe2-trans-nx-6HF

M062X/6311pp2d2p/H2O optimized

0 1

C	4.39069366	0.46116794	-0.98773858
C	3.25327570	0.02641246	-0.11882976
O	3.02942393	-1.19642377	0.08606940
H	4.98369569	1.22307547	-0.48537122
N	2.48329496	0.95762128	0.41835266
C	1.36069332	0.64220101	1.29704706
C	0.21870026	0.00348387	0.51807795
O	0.22285673	-0.03074196	-0.73866530
C	0.95539959	2.01922119	1.85502107
C	1.31012303	2.96227978	0.70432717
C	2.64125861	2.41150635	0.20740132
H	2.82700930	2.61810463	-0.84169992
H	1.67960419	-0.04594501	2.07756121
H	1.56659293	2.23427889	2.73011602
H	1.38783619	3.99906628	1.01736042
H	3.47502291	2.77401141	0.80908243
H	-0.09272371	2.05901798	2.13864468
H	0.56127845	2.89175381	-0.08704781
N	-0.80127874	-0.47478954	1.19890584
C	-1.95332306	-1.06284634	0.50558938
C	-2.55077454	-0.07847724	-0.48680930
O	-2.48531727	1.15527558	-0.23415470
C	-2.92291244	-1.38488214	1.65338675
C	-1.97760617	-1.70409022	2.81074286
C	-0.87627501	-0.65782859	2.66275223
H	-1.15428404	0.28554935	3.12911504
H	-1.62895686	-1.97006027	-0.00264123
H	-3.59094773	-2.20232590	1.39838396
H	-1.55752357	-2.70178625	2.68832277
H	0.07968497	-1.00148823	3.04488502
H	-3.51830049	-0.50119004	1.88576885
H	-2.46514193	-1.64344748	3.77913645
N	-3.16558263	-0.54794329	-1.55007658
C	-3.78672226	0.35788192	-2.51619029
H	-4.78191668	-0.01257215	-2.74689535
H	-3.19069373	0.38158066	-3.42728906
H	-3.85882249	1.35387654	-2.09785801
C	-3.23741458	-1.98088125	-1.86345105
H	-2.27923396	-2.34180242	-2.22944945
H	-3.98917085	-2.11037561	-2.63441338
H	-3.54489775	-2.55145271	-0.99187349
F	-1.62769495	2.84936927	-1.89492776
H	-1.96087477	2.20786901	-1.27492878
F	-2.39309047	2.02334841	2.08218448

H	-2.40530208	1.67609639	1.18113932
H	3.98510420	0.89241673	-1.90316967
H	5.01233886	-0.39381501	-1.23088300
F	1.57577653	1.25408399	-2.41846406
H	1.07857955	0.79617550	-1.74245632
F	4.49247725	-2.87843364	-1.01158156
H	3.92690288	-2.22313507	-0.58908209
F	-0.00956259	-2.24864880	-1.95369896
H	0.07754633	-1.41189910	-1.51344696
F	1.36980118	-2.48438200	1.43726057
H	2.00679282	-1.97960279	0.92780580

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Ac-Pro2-NMe2-trans-nx-HF212

M062X/6311pp2d2p/H2O optimized

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C	4.36654675	-0.91955304	0.71171575
C	3.24148518	-0.09600564	0.17015984
O	3.06946635	1.09193272	0.55701613
H	4.91448376	-1.39928979	-0.09701870
N	2.43044133	-0.64696654	-0.71463782
C	1.31608603	0.07375093	-1.32232855
C	0.17648526	0.25676582	-0.32708071
O	0.14282944	-0.33084104	0.76723664
C	0.88875100	-0.85569389	-2.47238256
C	1.19329700	-2.24339421	-1.90472967
C	2.52794494	-2.04013630	-1.19490501
H	2.67632820	-2.71327183	-0.35595305
H	1.64767533	1.04812334	-1.67388902
H	1.51340678	-0.64818832	-3.34000836
H	1.25425413	-3.00962186	-2.67191280
H	3.36572607	-2.12427062	-1.88753308
H	-0.15410421	-0.71947919	-2.74667992
H	0.42750188	-2.53185890	-1.18238446
N	-0.83090952	1.03773939	-0.69545138
C	-1.94123055	1.24879552	0.23114580
C	-2.56194621	-0.07754142	0.62917925
O	-2.64351111	-0.99320534	-0.23548352
C	-2.90674007	2.12965028	-0.57409740
C	-1.95494634	2.94888376	-1.44775706
C	-0.89086636	1.93465868	-1.86258005
H	-1.19546091	1.36951642	-2.74201958
H	-1.56536324	1.77309182	1.10749403
H	-3.53575684	2.73425972	0.07325096
H	-1.49565279	3.74155979	-0.85770802
H	0.07622664	2.39876387	-2.03142689
H	-3.54238572	1.49911127	-1.19688491
H	-2.45008189	3.39391131	-2.30583708
N	-3.04074103	-0.22636809	1.84559078
C	-3.68173214	-1.47839909	2.24544299
H	-4.57910201	-1.24175869	2.81044650
H	-3.00280530	-2.05677161	2.87084188
H	-3.94690829	-2.05223137	1.36609088
C	-2.87355739	0.78792919	2.89172033
H	-1.83059291	0.85597812	3.19595113
H	-3.46863737	0.48447028	3.74604085
H	-3.22939496	1.75721324	2.55423531
F	-1.68303431	-3.26067434	0.30534533
H	-2.05944350	-2.40737388	0.10581305
F	-2.51012566	-0.61938643	-2.67318083
H	-2.53497159	-0.73914253	-1.71315485
H	3.94753105	-1.69778223	1.34995976
H	5.03336335	-0.29078219	1.29193664
F	1.55586952	-2.07964006	1.74655237
H	1.02807667	-1.38526008	1.31939249
F	4.66609671	2.05879786	2.18848139
H	4.04603470	1.67616639	1.55588412
F	1.39070592	2.87805855	0.07812268
H	2.02516763	2.17832997	0.24750189

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Ac-Pro2-NMe2-trans-nx-HF221

M062X/6311pp2d2p/H2O optimized

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C	4.39127241	-0.48460049	-0.92371428
C	3.20742656	-0.19286530	-0.05659191
O	2.88371116	-0.97642522	0.87553068
H	5.04744068	0.38261357	-0.97518784
N	2.50797235	0.90245250	-0.29991046
C	1.35392308	1.29948492	0.50260147
C	0.16151641	0.38583547	0.24266730
O	0.18429246	-0.45950762	-0.68670101
C	1.08265538	2.74118436	0.03502975
C	1.53167210	2.70713624	-1.42649396
C	2.80255429	1.86752313	-1.37845724
H	3.00434463	1.34095554	-2.30569519
H	1.60388228	1.24705719	1.56040921
H	1.71106885	3.41651141	0.61350356
H	1.71035350	3.69638864	-1.83701852

H	3.66810856	2.46815978	-1.09792702
H	0.04218907	3.02791955	0.15928124
H	0.78013817	2.20736174	-2.04025537
N	-0.90204109	0.53029046	1.00412999
C	-2.07908618	-0.32923988	0.81912481
C	-2.64173999	-0.18944407	-0.59105017
O	-2.53036002	0.89545593	-1.19372834
C	-3.05797731	0.18677355	1.88298674
C	-2.12662567	0.66092396	2.99753848
C	-0.99320023	1.34011253	2.23485996
H	-1.24504650	2.36569079	1.97101177
H	-1.77894534	-1.35549992	1.02072954
H	-3.75668356	-0.58459818	2.19458489
H	-1.73756305	-0.19360678	3.55030388
H	-0.05244540	1.30961076	2.77511272
H	-3.61947530	1.02951915	1.47742909
H	-2.61090580	1.33998344	3.69300206
N	-3.26885584	-1.22140260	-1.13886104
C	-3.80383886	-1.09570388	-2.49114421
H	-4.85685309	-0.81578423	-2.45606546
H	-3.70782531	-2.06048678	-2.98378898
H	-3.24641430	-0.34503506	-3.03803081
C	-3.60506015	-2.47267468	-0.46910184
H	-3.08010893	-3.29616155	-0.94780959
H	-4.67984295	-2.62663945	-0.55648531
H	-3.34891205	-2.45035606	0.58217402
F	-2.19005269	3.04151880	-0.11218314
H	-2.29117636	2.15743454	-0.52859337
H	4.04263993	-0.70831013	-1.93208008
H	4.93279136	-1.33628291	-0.52676739
F	1.63811245	-0.61166605	-2.71601439
H	1.11192478	-0.51435365	-1.92140601
F	4.25914148	-3.01046165	1.25451400
H	3.72737537	-2.22175176	1.10209738
F	-0.61938306	-2.85677965	-0.54843372
H	-0.33549494	-1.95087246	-0.60315821
F	1.04693254	-1.03321718	2.56135636
H	1.75105150	-0.99625802	1.90962830

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Ac-Pro2-NMe2-trans-nx-HF3

M062X/6311pp2d2p/H2O optimized

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C	-4.53566189	-0.64657304	-1.39793351
C	-3.31707040	0.21965499	-1.22208759
O	-2.77315590	0.80030328	-2.15971286
H	-5.31285989	-0.37848173	-0.68339640
N	-2.83134050	0.32719503	0.03214136
C	-1.66175248	1.14231489	0.29350930
C	-0.41201924	0.52748692	-0.31789721
O	-0.34029703	-0.67219257	-0.63577245
C	-1.56261311	1.13869293	1.83127923
C	-2.16519841	-0.21843520	2.20543013
C	-3.33101323	-0.36101309	1.22896689
H	-3.56299483	-1.39759146	1.00057697
H	-1.79875197	2.14196411	-0.11202566
H	-2.17684009	1.94946801	2.22111975
H	-2.48718893	-0.26464332	3.24227140
H	-4.22717233	0.13717620	1.60436995
H	-0.54220851	1.27607663	2.18288406
H	-1.43759757	-1.01231359	2.03078447
N	0.66109799	1.30553159	-0.43546661
C	1.92030942	0.73749974	-0.91964939
C	2.27010290	-0.51950699	-0.14426414
O	2.12059002	-0.51438064	1.10977187
C	2.93368885	1.86401012	-0.66838851
C	2.08489681	3.12528239	-0.83466891
C	0.75393957	2.75450144	-0.18106109
H	0.76671370	2.93942120	0.89201904
H	1.82743791	0.52532626	-1.98117522
H	3.77150585	1.80904701	-1.35759711
H	1.93070167	3.33457207	-1.89254068
H	-0.08515007	3.27548045	-0.63361796
H	3.30969304	1.79586027	0.35219211
H	2.53617195	3.99734339	-0.37035000
N	2.76810624	-1.55994283	-0.77658131
C	3.18203430	-2.74954640	-0.03329735
H	4.10184049	-3.12639569	-0.47182241
H	2.40908759	-3.51452901	-0.09948560

H	3.35385552	-2.49325435	1.00511359
C	2.81970004	-1.64889605	-2.24017093
H	1.81944923	-1.57444088	-2.66138349
H	3.23415347	-2.61741479	-2.49713955
H	3.46191112	-0.87695095	-2.65656291
F	0.83625289	-2.40811677	2.16588668
H	1.33127500	-1.69533348	1.76843039
F	1.82060187	1.50763675	2.48553342
H	1.92324552	0.72926705	1.91750488
H	-4.26169516	-1.68732819	-1.22356118
H	-4.90727465	-0.53044324	-2.41042069
F	-1.96009731	-2.50206888	-0.48470417
H	-1.36632679	-1.73110506	-0.52017916

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Ac-Pro2-NMe2-trans-nx

M062X/6311pp2d2p/H2O optimized

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C	-4.43875499	-0.83217363	-1.66448014
C	-3.33343167	0.07560466	-1.18758779
O	-2.88051971	0.98012017	-1.88840468
H	-5.22152123	-0.93426015	-0.91435698
N	-2.85985771	-0.15429476	0.05109633
C	-1.75542244	0.62809606	0.57219139
C	-0.44749798	0.25420325	-0.12606575
O	-0.32097492	-0.80516797	-0.73171524
C	-1.69788371	0.20756982	2.05043850
C	-2.15293936	-1.25370084	2.00280683
C	-3.25521638	-1.25054446	0.94328782
H	-3.31272164	-2.19237883	0.40145083
H	-1.95941125	1.68760812	0.44481611
H	-2.40154343	0.81165094	2.62215600
H	-2.50928681	-1.61753257	2.96274195
H	-4.23122245	-1.04253744	1.38599799
H	-0.70410850	0.33033051	2.47543654
H	-1.32941760	-1.88623270	1.67456169
N	0.57800058	1.11151975	0.01847116
C	1.90240048	0.71811677	-0.44648895
C	2.35027039	-0.56312365	0.26536971
O	1.96267429	-0.78728882	1.40739405
C	2.80224462	1.90392754	-0.04560877
C	1.82602515	3.07151141	0.11236170
C	0.59060549	2.40323343	0.70761444
H	0.70112255	2.26273242	1.78589806
H	1.86725830	0.57400348	-1.52398546
H	3.58193787	2.08977560	-0.77973865
H	1.57808328	3.49332087	-0.86138629
H	-0.32025540	2.96231663	0.51480942
H	3.27570855	1.68905804	0.91286551
H	2.21490300	3.86307028	0.74729522
N	3.21363961	-1.36007465	-0.39307912
C	3.63372238	-2.62173224	0.19540354
H	4.71471657	-2.62941399	0.33554546
H	3.36188421	-3.44347404	-0.46812072
H	3.14259658	-2.75096310	1.15240531
C	3.69470927	-1.10123750	-1.74401632
H	3.00126186	-1.48077590	-2.49632155
H	4.64849080	-1.60949678	-1.86472595
H	3.86607874	-0.04213284	-1.90954567
H	-4.03581094	-1.82654507	-1.86098893
H	-4.85364511	-0.42798665	-2.58177866

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Ac-Pro2-NMe2-trans-nx-P2HFHF

M062X/6311pp2d2p/H2O optimized

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C	-4.57314092	-0.86192289	-1.63814128
C	-3.49759547	0.10362232	-1.21053951
O	-3.11356817	1.02204860	-1.93343546
H	-5.32751434	-0.98364175	-0.86222434
N	-2.96949999	-0.09025715	0.01313197
C	-1.88143580	0.74427514	0.48219919
C	-0.59248507	0.41672141	-0.26976841
O	-0.44600048	-0.63046335	-0.89249083
C	-1.75063827	0.34605488	1.96195996
C	-2.12752851	-1.13795584	1.94083894
C	-3.26879416	-1.20201495	0.92384890
H	-3.29357716	-2.14835363	0.38756930
H	-2.12952509	1.79429519	0.34988776
H	-2.47257163	0.91712453	2.54502383
H	-2.42741352	-1.51190740	2.91600649
H	-4.23751128	-1.04564595	1.40197958
H	-0.75426869	0.53477467	2.35669591
H	-1.28354317	-1.72859177	1.58641671
N	0.41453885	1.30172986	-0.14880635
C	1.70273343	0.99321004	-0.75889148
C	2.18026821	-0.38133610	-0.33103059
O	2.07045825	-0.70577303	0.88463633
C	2.62205847	2.10303146	-0.22556643
C	1.66200845	3.28183828	-0.05560480
C	0.38512352	2.63162605	0.47809280
H	0.40898858	2.53432911	1.56304441
H	1.61396300	1.04704151	-1.84097324
H	3.44466795	2.30463483	-0.90600326
H	1.46500035	3.74359065	-1.02269806
H	-0.50594613	3.17905508	0.18215751
H	3.02777560	1.80791447	0.74204907
H	2.04685467	4.04122346	0.61934805
N	2.76049186	-1.17766233	-1.20441024
C	3.31319214	-2.45931603	-0.76728549
H	4.17762112	-2.68887988	-1.38258638
H	2.56970746	-3.24834153	-0.87536505
H	3.61823517	-2.39059652	0.27090326
C	2.75417771	-0.90676769	-2.64593522
H	1.73319476	-0.81206040	-3.00884600

H	3.22369911	-1.74828522	-3.14288525
H	3.31945600	-0.00767068	-2.87904811
F	1.33316527	-2.96707323	1.65770576
H	1.63490995	-2.11244685	1.34620458
F	1.60638290	0.83910921	2.74788015
H	1.76368856	0.26022005	1.98636596
H	-4.13208664	-1.84116870	-1.82827438
H	-5.03323259	-0.49450398	-2.54916878

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Ac-Pro2-NMe2-trans-xn-4HF

M062X/6311pp2d2p/H2O optimized

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C	-4.57551977	0.76927077	-0.83726326
C	-3.31932356	0.51131221	-0.06058798
O	-2.73242484	1.40551522	0.58482502
H	-5.41519398	0.26581829	-0.35774189
N	-2.82065100	-0.72083520	-0.06924312

C	-1.58909000	-1.03625029	0.64854089
C	-0.45602233	-0.13020916	0.19975554
O	-0.35705225	0.25845386	-0.97541711
C	-1.31964712	-2.50341783	0.26697812
C	-2.71697496	-3.05127392	-0.02814457
C	-3.40077794	-1.89015578	-0.74293002
H	-3.14823115	-1.86097056	-1.80387154
H	-1.75682338	-0.91899711	1.71830164
H	-0.79097596	-3.03233993	1.05347081
H	-3.23965192	-3.27175472	0.90222201
H	-4.48126211	-1.89717282	-0.63102223
H	-0.70788680	-2.53168224	-0.63582114
H	-2.69431143	-3.95122178	-0.63619542
N	0.47129529	0.20004029	1.09242830
C	1.52695163	1.13324175	0.71742659
C	2.48138639	0.51014479	-0.29228005
O	2.61170780	-0.73928644	-0.34751986
C	2.22921277	1.43629226	2.05694560
C	1.95628002	0.18320054	2.89266453
C	0.52742952	-0.18919422	2.51263475
H	0.33006956	-1.25095919	2.62370665
H	1.07283524	2.01449528	0.27205744
H	1.75976723	2.30845469	2.50898842
H	2.06382667	0.35965751	3.95886056
H	-0.20180687	0.38932067	3.08144379
H	3.28935326	1.64230917	1.93013977
H	2.63085370	-0.62136495	2.60142831
N	3.17526053	1.30889995	-1.07837220
C	4.03928312	0.73343541	-2.10869781
H	4.98925979	0.41649727	-1.68073389
H	4.21622221	1.49335614	-2.86305731
H	3.54879181	-0.11915499	-2.56900727
C	3.14919928	2.76893414	-0.98597923
H	2.44408647	3.18361564	-1.70502777
H	4.14687015	3.13491655	-1.21141549
H	2.89325944	3.09727818	0.01465735
F	4.42428744	-2.24812759	-1.23442056
H	3.76332572	-1.62976601	-0.93262344
F	1.69767152	-2.55718536	1.08453417
H	1.98929942	-1.81083884	0.55440123
H	-4.47149703	0.37929438	-1.84808661
H	-4.76804110	1.83672410	-0.86683673
F	-2.02031461	0.16830177	-2.77415329
H	-1.38682385	0.16415945	-2.03459823
F	-3.65101865	3.64719691	0.57304124
H	-3.28444811	2.73247384	0.57217319

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Ac-Pro2-NMe2-trans-xn-5HF

M062X/6311pp2d2p/H2O optimized

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C	-4.58734346	0.88133635	-0.81733063
C	-3.33108910	0.63383391	-0.03870841
O	-2.69180187	1.54868002	0.52033959
H	-5.43789796	0.45014989	-0.28917350
N	-2.88471153	-0.61702015	0.04986913
C	-1.67767170	-0.92150734	0.80968061
C	-0.49500989	-0.11933193	0.30516068
O	-0.39321086	0.13794054	-0.91768981
C	-1.47063435	-2.42755787	0.56402330
C	-2.89315891	-2.93546112	0.32270703
C	-3.52720622	-1.81878562	-0.50097411
H	-3.28577006	-1.90867642	-1.56088106
H	-1.85115846	-0.70375074	1.86176035
H	-0.96229016	-2.90372207	1.39614378
H	-3.41966129	-3.04078713	1.27076509
H	-4.60559965	-1.76173706	-0.38326152
H	-0.86596303	-2.56447950	-0.33398909
H	-2.91352169	-3.88960384	-0.19587815
N	0.43620671	0.23437010	1.17078404
C	1.59120032	1.03403972	0.76446776
C	2.58507271	0.19572171	-0.04056489
O	2.42454045	-1.04966386	-0.12666531
C	2.17872806	1.50903429	2.10593728
C	1.81316015	0.37223640	3.06094517
C	0.40061221	-0.00347766	2.63133200
H	0.16194943	-1.04139651	2.83999764
H	1.24711618	1.85798523	0.14379817
H	1.68172900	2.43240273	2.39887262
H	1.85483449	0.66867555	4.10466153
H	-0.34270010	0.65475646	3.08158313

H	3.24780523	1.69257131	2.04523533
H	2.47850051	-0.47847150	2.91173363
N	3.60849155	0.79606117	-0.60980732
C	4.57150082	0.00744238	-1.37571788
H	4.72250356	-0.95652118	-0.90131784
H	5.51028745	0.55240216	-1.40105161
H	4.20763610	-0.13866511	-2.39257971
C	3.77684577	2.24188148	-0.71231783
H	3.72711662	2.52286207	-1.76316229
H	4.75019948	2.51344118	-0.30884721
H	3.00980669	2.77821663	-0.16974034
F	2.73282982	-2.45372089	-2.20072125
H	2.64787329	-1.90891492	-1.42346701
F	1.53143268	-2.59040441	1.61861284
H	1.83881851	-1.97177996	0.95273862
H	-4.51491431	0.40893258	-1.79528864
H	-4.73846316	1.95003183	-0.92924771
F	-2.12056196	0.00559718	-2.74676773
H	-1.50785803	0.00489713	-2.01364641
F	-3.48807216	3.83331316	0.31379051
H	-3.17214658	2.90608079	0.39358644
F	1.28096758	1.32895257	-2.35240013
H	0.65623707	0.87550230	-1.78760956

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Ac-Pro2-NMe2-trans-xn-6HF

M062X/6311pp2d2p/H2O optimized

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C	4.54256023	-0.44816155	-1.10235587
C	3.31412362	-0.40867959	-0.24672448
O	2.76922470	-1.47243395	0.14533185
H	5.40910320	-0.15755903	-0.50751957
N	2.81869063	0.77279705	0.08352766
C	1.62267959	0.92754836	0.91122246
C	0.42477918	0.21707309	0.31222996
O	0.34980254	0.04165331	-0.92671652
C	1.39902663	2.45305340	0.93505886
C	2.81010733	3.01153148	0.76272112
C	3.43148240	2.07003277	-0.26069377
H	3.15556562	2.33601176	-1.28139726
H	1.82310697	0.53632629	1.90834316
H	0.90235661	2.77358229	1.84485302
H	3.35661921	2.95100065	1.70313028
H	4.51245582	2.00788165	-0.18322152
H	0.77444352	2.73653080	0.08655923
H	2.81178459	4.04278881	0.42222492
N	-0.53211484	-0.16633171	1.13288094
C	-1.65352722	-0.97847487	0.66254156
C	-2.65490782	-0.13255845	-0.12185936
O	-2.52744416	1.11977017	-0.14864391
C	-2.24979558	-1.54291902	1.96496174
C	-1.91993929	-0.45971889	2.99204843
C	-0.50682885	-0.04421517	2.60620718
H	-0.27079637	0.97473597	2.89536145
H	-1.26194954	-1.75990931	0.01447396
H	-1.73315081	-2.46978021	2.20732588
H	-1.97209651	-0.81943466	4.01511186
H	0.23077344	-0.74036980	3.00573161
H	-3.31403946	-1.74301531	1.87738588
H	-2.59523994	0.38921839	2.88329310
N	-3.65003605	-0.73440315	-0.73807214
C	-4.62208365	0.05798463	-1.48792149
H	-4.79057477	1.00692248	-0.99014215
H	-5.55202684	-0.50110162	-1.53152415
H	-4.25617757	0.23541233	-2.49907703
C	-3.77549487	-2.17856184	-0.90448811
H	-3.69638398	-2.41401288	-1.96479061
H	-4.74895322	-2.49360737	-0.53416385
H	-3.00504885	-2.71598674	-0.36765957
F	-2.81604502	2.57423240	-2.18801411
H	-2.73767252	2.01170876	-1.42224691
F	-1.64721049	2.57326054	1.67622383
H	-1.94941344	1.98782661	0.97771779
H	4.44298805	0.24730243	-1.93248605
H	4.69022471	-1.45580478	-1.47619241
F	1.97820620	0.68377920	-2.74105493
H	1.39313867	0.47613802	-2.01529894
F	3.79970494	-3.63360334	-0.51730772
H	3.40960576	-2.78820050	-0.26819345

F	-1.27518530	-1.11093469	-2.46541222
H	-0.67289044	-0.67615237	-1.86670469
F	0.84277477	-2.61271344	1.34875028
H	1.54250918	-2.12459641	0.93462395

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Ac-Pro2-NMe2-trans-xn-HF212

M062X/6311pp2d2p/H2O optimized

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C	4.54388580	-0.15610953	-1.18319035
C	3.31478308	-0.25779242	-0.33377523
O	2.86115451	-1.38337281	0.00266473
H	5.38053673	0.18564369	-0.57298151
N	2.72652068	0.85881806	0.05776597
C	1.52003344	0.87173507	0.88414278
C	0.36796993	0.14905759	0.20785013
O	0.30620934	0.01038799	-1.02365385
C	1.20320224	2.37367902	1.03980762
C	2.56590838	3.04311671	0.86965676
C	3.21803177	2.21742681	-0.23136911
H	2.87663872	2.51728557	-1.22309325
H	1.73764119	0.40387338	1.84467873
H	0.71915263	2.58641114	1.98741167
H	3.14621771	2.95922030	1.78791453
H	4.30259059	2.24254623	-0.20031049
H	0.52894898	2.68236163	0.24024387
H	2.48508415	4.09237747	0.60093704
N	-0.60480594	-0.30081274	0.99132624
C	-1.64515412	-1.14979492	0.42463663
C	-2.64832080	-0.33060624	-0.37942304
O	-2.66821973	0.92185325	-0.26977467
C	-2.27962240	-1.81017584	1.66315408
C	-2.03514681	-0.78202338	2.76992141
C	-0.62944120	-0.27970032	2.46429405
H	-0.45115435	0.72537416	2.83390227
H	-1.17178926	-1.87224470	-0.23588899
H	-1.74036782	-2.73212632	1.87478382
H	-2.10905694	-1.21011366	3.76524671
H	0.12529675	-0.96707261	2.84839581
H	-3.33110739	-2.04354445	1.51619019
H	-2.74568036	0.04085943	2.68956239
N	-3.50860982	-0.95596082	-1.15889127
C	-4.50125973	-0.16689218	-1.88949773
H	-4.99076248	0.53071020	-1.21470072
H	-5.23752018	-0.84798361	-2.30277937
H	-4.02631354	0.38729418	-2.69713719
C	-3.56608412	-2.40125361	-1.36026481
H	-3.44873741	-2.61678507	-2.42052024
H	-4.53531755	-2.76690600	-1.02568612
H	-2.79047246	-2.91498533	-0.80777372
F	-3.52415425	2.80889635	-1.70034970
H	-3.23431566	2.05401606	-1.19404510
F	-1.86083712	2.34556691	1.61187245
H	-2.11377390	1.75143210	0.90104750
H	4.38490923	0.55769572	-1.98795633
H	4.77964526	-1.13233097	-1.59374536
F	1.89846108	0.69562734	-2.76309371
H	1.29069008	0.45002314	-2.04526497
F	4.06424403	-3.41414969	-0.75148099
H	3.60443230	-2.61483500	-0.46495279
F	0.98291694	-2.64375728	1.13383020
H	1.66130860	-2.10710872	0.73856194

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Ac-Pro2-NMe2-trans-xn-HF221

M062X/6311pp2d2p/H2O optimized

0 1

C	4.42593113	-0.99835233	-0.62616982
C	3.15800413	-0.57079053	0.04580719
O	2.50950357	-1.37327190	0.76552619
H	5.27453074	-0.50547074	-0.15149915
N	2.73772071	0.67040342	-0.13717222
C	1.51902467	1.19059697	0.48238859
C	0.29596919	0.38349901	0.08859143
O	0.27682467	-0.23542905	-1.00217627
C	1.42569796	2.63071551	-0.06116831
C	2.88314250	2.99524495	-0.33584789
C	3.46177399	1.70422190	-0.89992461
H	3.24116433	1.58571360	-1.96122359
H	1.63695641	1.17710605	1.56532607
H	0.92593886	3.29250498	0.63789586
H	3.39072358	3.25317931	0.59290866
H	4.53148422	1.61075724	-0.74140615
H	0.85446577	2.62715739	-0.98991472
H	2.98141217	3.82415257	-1.03065873
N	-0.73087915	0.38901375	0.91266419
C	-1.89118647	-0.47869140	0.70159989
C	-2.81725608	0.07840176	-0.38044448

O	-2.67451884	1.23611636	-0.81049036
C	-2.57016728	-0.48750659	2.08443829
C	-2.21800122	0.88850037	2.64779357
C	-0.76577048	1.06513640	2.22738505
H	-0.47820774	2.10638338	2.12355086
H	-1.53489502	-1.46367951	0.40667342
H	-2.12108145	-1.27407957	2.68826858
H	-2.33868157	0.94710356	3.72535611
H	-0.09343838	0.54515281	2.91038367
H	-3.64065804	-0.65863607	2.01545384
H	-2.83189299	1.66049544	2.18299266
N	-3.79407593	-0.71100741	-0.81668583
C	-4.63062193	-0.25588443	-1.92082151
H	-4.70235006	0.82491417	-1.90524286
H	-5.61945603	-0.69294140	-1.81072543
H	-4.19802992	-0.57897116	-2.86928833
C	-3.89192419	-2.13322879	-0.50730046
H	-3.37168397	-2.71583537	-1.26769807
H	-4.94380339	-2.40732934	-0.49823833
H	-3.47914402	-2.36103648	0.46846804
F	-1.59243955	3.15879957	0.23258088
H	-1.98609984	2.35861033	-0.16389577
H	4.40359981	-0.71550480	-1.67650201
H	4.54031493	-2.07312034	-0.53266421
F	2.06165568	-0.49032080	-2.76411919
H	1.41979885	-0.34832321	-2.07092813
F	3.38035283	-3.68349347	1.03314353
H	3.05328091	-2.78348118	0.92058870
F	-1.39710169	-1.56366435	-2.31629557
H	-0.79386437	-1.05037626	-1.78342329
F	0.43630438	-1.87712703	2.14468227
H	1.18914108	-1.61155908	1.63303392

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Ac-Pro2-NMe2-trans-xn-HF3

M062X/6311pp2d2p/H2O optimized

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C	4.59993921	-1.78447370	0.14819617
C	3.36871372	-1.05539671	0.61571601
O	2.65645671	-1.46867001	1.53017079
H	5.49327308	-1.20722071	0.38756232
N	3.06631751	0.09121026	-0.02467411
C	1.88308937	0.84708611	0.35512602
C	0.63968090	-0.01955784	0.27270646
O	0.50107128	-0.88629634	-0.60620945
C	1.84110115	1.99147499	-0.67437427
C	3.31161742	2.16500244	-1.06034030
C	3.83104410	0.73059173	-1.09883498
H	3.61162224	0.24678096	-2.05244603
H	1.99824452	1.22397556	1.37112942
H	1.37966583	2.88479722	-0.26588797
H	3.83739449	2.72597574	-0.28771384
H	4.89828022	0.66334983	-0.90431860
H	1.26040194	1.67350960	-1.54149453
H	3.43841507	2.67739673	-2.01014116
N	-0.34302300	0.20735218	1.14046383
C	-1.50994095	-0.66604182	1.14839711
C	-2.35228988	-0.46918487	-0.10451945
O	-2.34675857	0.64196021	-0.69471920
C	-2.27037718	-0.23629965	2.41945088
C	-1.83840101	1.21938610	2.61819436
C	-0.36634274	1.20698052	2.22151797
H	-0.02481258	2.17015436	1.85482877
H	-1.17355094	-1.69832243	1.18792090
H	-1.93493321	-0.85260875	3.25189882
H	-1.98547837	1.56372978	3.63769507
H	0.26710049	0.87467476	3.04530872
H	-3.34683713	-0.35227112	2.31710553
H	-2.39117182	1.87404219	1.94479773
N	-3.09488230	-1.47100741	-0.53146368
C	-3.84135290	-1.34224796	-1.78217072
H	-4.80846187	-0.87310111	-1.60700978
H	-3.98985466	-2.33796825	-2.18885670
H	-3.27344460	-0.74768210	-2.49069893
C	-3.23359905	-2.74284652	0.17901029
H	-2.53388149	-3.47803711	-0.21641164
H	-4.24884874	-3.09913318	0.02868947
H	-3.07853987	-2.61960538	1.24472816
F	-4.07466003	1.76340545	-2.13712538

H	-3.44206694	1.28741475	-1.60242165
F	-1.15028150	2.77353969	-0.22636311
H	-1.55827771	1.91347629	-0.35718706
H	4.56449421	-1.92607662	-0.93105622
H	4.64940596	-2.74560758	0.64870469
F	2.17765861	-1.82511596	-2.12862216
H	1.55507431	-1.40377920	-1.50840232

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Ac-Pro2-NMe2-trans-xn

M062X/6311pp2d2p/H2O optimized

0 1

C	4.37236866	-0.37511934	2.04313727
C	3.17464053	0.21700569	1.34357988
O	2.46245836	1.07033622	1.87209708
H	5.29092953	-0.01456490	1.57908572

N	2.91848750	-0.22489884	0.09896038
C	1.78039662	0.29846514	-0.64242656
C	0.47011385	0.01371416	0.08341130
O	0.31542674	-1.01430957	0.73442733
C	1.83701606	-0.46770139	-1.97685163
C	3.31579506	-0.83691779	-2.11392018
C	3.71452403	-1.17528841	-0.68020247
H	3.44167267	-2.20233384	-0.42566405
H	1.90809905	1.37110396	-0.78775935
H	1.45851300	0.12483024	-2.80569142
H	3.88818634	0.02451701	-2.45805555
H	4.77606330	-1.03763959	-0.49244438
H	1.23540722	-1.37378866	-1.89417351
H	3.48397232	-1.66354534	-2.79898818
N	-0.51469733	0.91150934	-0.07795997
C	-1.81846551	0.65557223	0.50752066
C	-2.52418152	-0.48230939	-0.24497120
O	-2.17727962	-0.78050228	-1.38289274
C	-2.55193526	1.99264356	0.31089303
C	-1.96182871	2.51369934	-1.00196305
C	-0.48652597	2.12321580	-0.90949969
H	-0.05515677	1.92017551	-1.88748703
H	-1.69489595	0.38916309	1.55374633
H	-2.30292093	2.66009288	1.13540349
H	-2.09403545	3.58452241	-1.13039416
H	0.09980384	2.90186194	-0.41836180
H	-3.63259465	1.87547189	0.27362317
H	-2.42476579	2.00181092	-1.84434773
N	-3.55112189	-1.08118408	0.39331482
C	-4.23754678	-2.20485347	-0.22296068
H	-5.28696826	-1.95954325	-0.38849222
H	-4.18255001	-3.07240268	0.43564193
H	-3.76532865	-2.43702485	-1.16985006
C	-3.97347066	-0.76338736	1.75030857
H	-3.46058052	-1.39037944	2.48200325
H	-5.04316148	-0.94863949	1.82551978
H	-3.80343453	0.28062641	1.99043866
H	4.36978169	-1.46208396	1.97745939
H	4.35503990	-0.06684280	3.08319614

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Ac-Pro2-NMe2-trans-xn-P2HFHF

M062X/6311pp2d2p/H2O optimized

0 1

C	4.69992630	-1.69735272	-1.16356862
C	3.51483201	-1.29178211	-0.32410090
O	2.88841235	-2.09889335	0.36247675
H	5.61680480	-1.28810906	-0.73860187
N	3.16778151	0.00806914	-0.35074758
C	2.03428187	0.47412014	0.43465480
C	0.75298392	-0.22694479	-0.00149109
O	0.55961793	-0.54298428	-1.16914034
C	1.97597973	1.98257089	0.12986564
C	3.41411774	2.32191175	-0.26768098
C	3.84915420	1.09271617	-1.06007686
H	3.50465424	1.14732268	-2.09562538
H	2.22569563	0.28233556	1.49011319
H	1.60579002	2.55195970	0.97689106
H	4.03683910	2.42092177	0.62158147
H	4.92546088	0.94340538	-1.05515074
H	1.30444565	2.15289964	-0.71259535
H	3.48629167	3.23817841	-0.84770222
N	-0.18354238	-0.43054715	0.94550521
C	-1.38580027	-1.16914500	0.60042535
C	-2.28838317	-0.35868114	-0.32133041
O	-2.22324900	0.89734259	-0.31987581
C	-2.05220710	-1.43249475	1.96636738
C	-1.53884836	-0.28355693	2.83855033
C	-0.09498917	-0.11229466	2.37760161
H	0.26822481	0.90123271	2.52251159
H	-1.10631855	-2.08586629	0.08726069
H	-1.69738925	-2.38870356	2.34811807
H	-1.61028504	-0.49982226	3.90077150
H	0.56953333	-0.81770825	2.88058877
H	-3.13722765	-1.46909926	1.90113334
H	-2.09741832	0.62892837	2.63036718
N	-3.14817033	-0.99477070	-1.09406811
C	-3.96640408	-0.23020005	-2.03423687
H	-4.78757183	0.26392366	-1.51687692
H	-4.36575564	-0.91844864	-2.77206590
H	-3.35637782	0.51671486	-2.53434882
C	-3.36056777	-2.44118347	-1.07137046
H	-2.83807309	-2.91459403	-1.90156181
H	-4.42729698	-2.62554237	-1.16924360
H	-3.03156998	-2.87500540	-0.13487591
F	-3.69091931	2.75412345	-1.15562066
H	-3.17034334	2.00333208	-0.87382425
F	-0.96314772	2.49418793	1.11644041
H	-1.37841795	1.80753520	0.58767560

H	4.60679314	-1.31961942	-2.18071770
H	4.76492836	-2.78005260	-1.17536463

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Ac-Pro2-NMe2-trans-xn

M062X/6311pp2d2p/H2O optimized

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C	4.40223235	0.07640933	2.04448202
C	3.20158638	0.50981550	1.24133913
O	2.50616827	1.47155391	1.56766789
H	5.31809710	0.29390040	1.49425471
N	2.92315511	-0.20180231	0.13405425
C	1.77718404	0.14981051	-0.69150756
C	0.47522490	0.03573452	0.09407607
O	0.32947594	-0.82141002	0.95965234
C	1.81412441	-0.89305408	-1.82415473
C	3.28671934	-1.30493898	-1.88536288
C	3.69398010	-1.31902018	-0.41459998

H	3.40256498	-2.25641789	0.06547654
H	1.90448625	1.16338148	-1.07097536
H	1.43506921	-0.49257643	-2.76091400
H	3.86686274	-0.55198623	-2.41873325
H	4.75966947	-1.16552071	-0.26765121
H	1.20238755	-1.75042063	-1.54079395
H	3.43644161	-2.26753641	-2.36717337
N	-0.51346248	0.87339303	-0.25528123
C	-1.81715673	0.74560684	0.37152998
C	-2.52848595	-0.51881591	-0.13612316
O	-2.17626713	-1.04751913	-1.18511011
C	-2.54676011	2.01645592	-0.09317583
C	-1.96368971	2.25050381	-1.48882685
C	-0.48944898	1.87687568	-1.32891891
H	-0.07241565	1.46320327	-2.24474951
H	-1.69325219	0.69631004	1.44978019
H	-2.29017743	2.83922698	0.57357360
H	-2.09105413	3.27223552	-1.83551036
H	0.10834884	2.73758526	-1.02449089
H	-3.62787992	1.89936482	-0.10020048
H	-2.43524003	1.57827279	-2.20404893
N	-3.56819871	-0.96224682	0.60100467
C	-4.26303807	-2.18189126	0.22161095
H	-5.32723266	-1.97970769	0.10097733
H	-4.13762207	-2.93692214	0.99915651
H	-3.85502227	-2.55209436	-0.71115000
C	-3.97123857	-0.38849259	1.87734126
H	-3.44875731	-0.86495876	2.70897952
H	-5.03965659	-0.55331485	2.00063492
H	-3.79734939	0.68156771	1.90933665
H	4.37778894	-0.99437388	2.24124759
H	4.41106842	0.62438170	2.98059192

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Ac-Pro2-NMe2-trans-xx-4HF

M062X/6311pp2d2p/H2O optimized

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C	-4.38693196	0.40597327	-0.98877153
C	-3.15281024	0.49559369	-0.14248926
O	-2.64752540	1.58687995	0.19537928
H	-5.22369945	0.06138343	-0.38055326
N	-2.58463906	-0.63717427	0.25892423
C	-1.37146519	-0.61694978	1.06533906
C	-0.24963713	0.12804179	0.37233496
O	-0.14420275	0.15038299	-0.86606452
C	-0.99666707	-2.10691271	1.19088052
C	-2.34642303	-2.81543223	1.06411275
C	-3.06669706	-1.99961926	-0.00582058
H	-2.77221475	-2.30042282	-1.01227765
H	-1.58353807	-0.17307712	2.03618009
H	-0.46963197	-2.30995952	2.11809302
H	-2.89249664	-2.75431940	2.00497673
H	-4.14863086	-2.04570123	0.08082110
H	-0.34854662	-2.38478191	0.35721999
H	-2.24680089	-3.86056408	0.78543425
N	0.70219968	0.65671288	1.13271266
C	1.90451533	1.20734468	0.50585702
C	2.49694518	0.20679436	-0.47060723
O	2.52804110	-1.01093727	-0.14112899
C	2.83811530	1.45707850	1.69978326
C	1.86092429	1.78723345	2.82850561
C	0.70410546	0.81526901	2.59963372
H	0.88699236	-0.14840172	3.07165041
H	1.64939947	2.13623379	0.00318773
H	3.55091878	2.25030656	1.49317760
H	1.50694266	2.81250453	2.72830456
H	-0.24580966	1.21987813	2.93750365
H	3.38507164	0.54281809	1.93139933
H	2.30277386	1.66650269	3.81337506
N	3.01299313	0.63069007	-1.60415589
C	3.65174764	-0.31528816	-2.51906852
H	4.51278627	0.16935327	-2.96984702
H	2.95101226	-0.61049732	-3.29940416
H	3.97457606	-1.19229236	-1.97041674
C	2.86497920	2.01261479	-2.07425906
H	1.81486616	2.25021330	-2.23223288
H	3.38734829	2.09777042	-3.02044356
H	3.30680929	2.71447632	-1.37178882
F	1.62182191	-2.72648516	-1.74683392
H	1.98179442	-2.07573894	-1.14839835
F	2.16700886	-1.88932679	2.14624933
H	2.28352209	-1.51856860	1.26242546
H	-4.23341957	-0.30441256	-1.79852526
H	-4.61926425	1.38669734	-1.39116450
F	-1.72314658	-0.62250703	-2.57750222
H	-1.12467269	-0.34284740	-1.86301065
F	-3.69042083	3.63646607	-0.56381889
H	-3.27204258	2.79746889	-0.25897230

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Ac-Pro2-NMe2-trans-xx-5HF

M062X/6311pp2d2p/H2O optimized

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C	-4.34747500	0.91288200	-0.69567800
C	-3.10706400	0.62971100	0.09615200
O	-2.46162900	1.52255800	0.68380500
H	-5.21019500	0.46447800	-0.20308700
N	-2.68191500	-0.62945100	0.15901100
C	-1.46229600	-0.96820200	0.88192500
C	-0.29650500	-0.12053600	0.42649400
O	-0.18588900	0.19852900	-0.78559100
C	-1.22386600	-2.44203700	0.50349900
C	-2.64369800	-2.96533700	0.27758300

C	-3.33694100	-1.80588900	-0.43410200
H	-3.15126700	-1.82112700	-1.50795400
H	-1.62317500	-0.85398500	1.95174100
H	-0.67174500	-2.96810900	1.27617800
H	-3.12829500	-3.15754600	1.23432700
H	-4.40787600	-1.77603300	-0.25294400
H	-0.65378700	-2.48640600	-0.42704000
H	-2.66374600	-3.87714100	-0.31229200
N	0.65142400	0.17558000	1.29246700
C	1.91668500	0.78358500	0.85876000
C	2.51439000	0.01202100	-0.30751900
O	2.32853200	-1.23417500	-0.37222800
C	2.79843900	0.67705200	2.11391200
C	1.78606000	0.80274300	3.25084300
C	0.59461000	-0.01423800	2.75915400
H	0.70468400	-1.07226500	2.98945000
H	1.73807900	1.82141200	0.58442500
H	3.56986400	1.44142900	2.13228400
H	1.49489000	1.84437000	3.37960300
H	-0.35008800	0.35808100	3.14402900
H	3.27358100	-0.30419500	2.13978200
H	2.16950400	0.42837800	4.19540400
N	3.25161700	0.65875100	-1.18270100
C	3.86922600	-0.04085000	-2.30852400
H	4.94151400	0.14003000	-2.28909800
H	3.45611400	0.34888900	-3.23730100
H	3.67693900	-1.10336000	-2.23662200
C	3.50080800	2.10433700	-1.11190700
H	2.61953500	2.65901200	-1.42449100
H	4.32387600	2.32610200	-1.78285100
H	3.79472400	2.39790000	-0.10843300
F	1.16301000	-2.26788800	-2.37169400
H	1.60069800	-1.86594400	-1.62951800
F	1.85901100	-2.62463600	1.62435300
H	2.02180100	-2.06997100	0.85211500
H	-4.25849900	0.47642900	-1.68952900
H	-4.49275500	1.98552100	-0.77064700
F	-1.77906600	-0.23020400	-2.67564800
H	-1.19200000	-0.12356700	-1.92660000
F	-3.17816600	3.83187400	0.45505700
H	-2.89515400	2.89536500	0.54518900
F	0.35625700	2.56924900	-1.41019400
H	0.15313400	1.66579000	-1.17587000

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Ac-Pro2-NMe2-trans-xx-6HF

M062X/6311pp2d2p/H2O optimized

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C	4.31214535	-0.28600028	-1.10872268
C	3.14375302	-0.23232714	-0.17562245
O	2.75351630	-1.26968236	0.42452591
H	5.16955277	0.19701765	-0.63890248
N	2.53003007	0.92516686	0.00138733
C	1.35384157	1.08143414	0.85713998
C	0.20746580	0.19156138	0.42361117
O	0.16170883	-0.29178735	-0.73703900
C	0.96236699	2.56214282	0.66700887
C	2.29044165	3.23012143	0.31874944
C	2.96149109	2.20700964	-0.58869281
H	2.59579153	2.26973504	-1.61411080
H	1.62016309	0.86919347	1.89170097
H	0.47996891	2.96530159	1.55178992
H	2.88676307	3.37561330	1.21885544
H	4.04454978	2.27768260	-0.58509562
H	0.26716833	2.64604209	-0.17040307
H	2.15857971	4.18895559	-0.17378673
N	-0.78920895	0.01323709	1.26435566
C	-1.98754749	-0.73046643	0.85479566
C	-2.56831866	-0.15863727	-0.42703070
O	-2.47411675	1.08130940	-0.63568827
C	-2.94071995	-0.53871523	2.04507384
C	-1.98160283	-0.43371474	3.23010284
C	-0.84243587	0.42138776	2.68428676
H	-1.07532088	1.48283386	2.74021243
H	-1.72194154	-1.77808401	0.72613518
H	-3.65050872	-1.35669682	2.12737592
H	-1.60630865	-1.42073620	3.49839146
H	0.10532708	0.21021441	3.16729188
H	-3.49059106	0.39523753	1.92240942

H	-2.44284836	0.01658736	4.10403509
N	-3.20421093	-0.96463576	-1.24871669
C	-3.83584907	-0.44384466	-2.46093543
H	-4.82054881	-0.89291921	-2.55760762
H	-3.23299123	-0.70466126	-3.32955589
H	-3.93378360	0.63256858	-2.39246054
C	-3.28782510	-2.41561840	-1.03401390
H	-2.31206409	-2.87955230	-1.15704013
H	-3.96865896	-2.81800120	-1.77579536
H	-3.68842089	-2.63746164	-0.04815912
F	-1.63503270	1.99590167	-2.83068355
H	-1.96482632	1.64600030	-2.00811727
F	-2.20841630	2.76885811	1.16441481
H	-2.29194735	2.09916408	0.47674309
H	4.08139820	0.23739885	-2.03345494
H	4.55909636	-1.32190598	-1.31689430
F	1.59100588	0.24640759	-2.73360284
H	1.06191632	0.08394701	-1.95367085
F	3.74724455	-3.46178738	-0.19401558
H	3.36670160	-2.61015333	0.04512438
F	-0.01952450	-2.82678933	-0.86447130
H	0.06628721	-1.88137316	-0.84597785
F	1.39270647	-1.66690637	2.47913461
H	1.91726846	-1.49419994	1.69590545

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Ac-Pro2-NMe2-trans-xx-HF212

M062X/6311pp2d2p/H2O optimized

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C	4.29758257	-0.62001245	1.03466306
C	3.14473962	0.01775956	0.32425537
O	2.84564079	1.22304840	0.54318751
H	5.11173324	-0.78578954	0.32874760
N	2.45194651	-0.70626665	-0.53618527
C	1.29000026	-0.18655063	-1.25646932
C	0.16616230	0.21125244	-0.31681797
O	0.11097517	-0.18906033	0.85857672
C	0.82777442	-1.38113571	-2.11963379
C	2.09107782	-2.22562763	-2.27272655
C	2.75543127	-2.09935356	-0.90762576
H	2.30904570	-2.76967769	-0.17161973
H	1.58908225	0.66251405	-1.86945295
H	0.40077876	-1.05167983	-3.06163792
H	2.74054837	-1.80340803	-3.03864302
H	3.82845117	-2.25813299	-0.93652481
H	0.06343588	-1.94242008	-1.57948753
H	1.87371481	-3.25895706	-2.52722038
N	-0.82873477	0.92254491	-0.82919814
C	-1.98637952	1.23828951	0.00787559
C	-2.56607657	-0.02915988	0.60876436
O	-2.62061830	-1.06609730	-0.10806813
C	-2.95620771	1.90806287	-0.97647344
C	-2.00863339	2.59627744	-1.96006161
C	-0.89346966	1.57019777	-2.15218485
H	-1.15848887	0.83105549	-2.90617449
H	-1.67607380	1.93003899	0.78720673
H	-3.63533102	2.58926398	-0.47181265
H	-1.60088119	3.50370333	-1.51538819
H	0.05904914	2.03303307	-2.38940711
H	-3.53901113	1.14304374	-1.49048277
H	-2.49203078	2.85246500	-2.89831385
N	-3.04260287	-0.00748306	1.83510232
C	-3.66437605	-1.20200111	2.40612949
H	-4.52219436	-0.89525122	2.99771364
H	-2.95127360	-1.72365317	3.04351241
H	-3.98984068	-1.86107231	1.61008350
C	-2.87045056	1.14158524	2.73076485
H	-1.81584551	1.30408209	2.94414479
H	-3.38431615	0.91713475	3.65854978
H	-3.30867742	2.03952411	2.30346655
F	-1.69028279	-3.21407061	0.82494019
H	-2.05875923	-2.40618067	0.47547223
F	-2.41160182	-1.11635907	-2.57635476
H	-2.46797104	-1.06530899	-1.61411873
H	3.99592692	-1.57857780	1.45042192
H	4.64158731	0.03754251	1.82610154
F	1.53636641	-1.77761537	2.07269053

H 0.99743855 -1.15574363 1.55714099
F 4.11685816 2.48726442 2.25568744
H 3.62646748 1.98968632 1.59030704
F 1.43537806 2.91382861 -0.62687932
H 1.96768064 2.24313804 -0.19369912

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Ac-Pro2-NMe2-trans-xx-HF221

M062X/6311pp2d2p/H2O optimized

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C -4.25857628 0.90430404 -0.74406594

C	-3.05946204	0.40967595	0.00220737
O	-2.55475065	1.09526914	0.93168799
H	-5.13124923	0.31653636	-0.45763997
N	-2.54154804	-0.75747629	-0.33900657
C	-1.34482784	-1.31399546	0.29296054
C	-0.14654274	-0.39561662	0.15546157
O	-0.12365765	0.50322842	-0.72414610
C	-1.09966084	-2.62268943	-0.48686002
C	-2.49740851	-3.01074591	-0.96419078
C	-3.11359006	-1.67097633	-1.34625558
H	-2.80257513	-1.34742498	-2.33996342
H	-1.54607928	-1.50884512	1.34520760
H	-0.61259936	-3.37059411	0.13087456
H	-3.06429203	-3.46210904	-0.15065128
H	-4.19731324	-1.66567121	-1.28668900
H	-0.45367079	-2.41620779	-1.34144744
H	-2.47486488	-3.70194117	-1.80153729
N	0.89615035	-0.61707638	0.92556054
C	2.11911592	0.18685510	0.78611517
C	2.63872169	0.14723190	-0.64708064
O	2.48545962	-0.88110155	-1.33252487
C	3.09170303	-0.48594951	1.76580074
C	2.16535116	-1.03526436	2.84968797
C	0.97755525	-1.56646917	2.05595515
H	1.16813661	-2.56378583	1.66382626
H	1.88971644	1.20735487	1.08685126
H	3.83434210	0.21238105	2.14168392
H	1.83873235	-0.23212871	3.50952347
H	0.05555536	-1.54782348	2.62687373
H	3.60394268	-1.30478053	1.25894465
H	2.63307802	-1.81254251	3.44689440
N	3.27543072	1.21170355	-1.11543964
C	3.74298838	1.22621211	-2.49750759
H	4.81309898	1.02312410	-2.53445660
H	3.55457756	2.21440019	-2.91186500
H	3.20921652	0.47861968	-3.07118377
C	3.61503481	2.39653155	-0.32947054
H	2.87522265	3.17993522	-0.48004661
H	4.58853074	2.74598444	-0.66504643
H	3.69433393	2.16371003	0.72628007
F	2.04082837	-3.09646743	-0.43278519
H	2.18655336	-2.18834758	-0.77077829
H	-4.10435923	0.79691208	-1.81550630
H	-4.43452570	1.94533193	-0.49403432
F	-1.65977964	0.85785671	-2.66500207
H	-1.09472641	0.67457918	-1.91251585
F	-3.42871280	3.38142341	1.35200386
H	-3.09526650	2.49259114	1.18747701
F	0.50363940	2.88655406	-0.16384513
H	0.27850582	1.98913207	-0.38669013
F	-1.05908173	0.56197366	2.85731936
H	-1.63311717	0.74569870	2.11191635

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Ac-Pro2-NMe2-trans-xx-HF3

M062X/6311pp2d2p/H2O optimized

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C	-4.38521744	-0.69361422	-1.69057647
C	-3.16644422	0.12097209	-1.34702825
O	-2.49972167	0.71201177	-2.19532050
H	-5.28100943	-0.22017500	-1.28841884
N	-2.82441225	0.17418817	-0.04406240
C	-1.64861505	0.91769968	0.37031100
C	-0.39472143	0.42194666	-0.31665825
O	-0.24844602	-0.77081233	-0.63724950
C	-1.54602053	0.62346882	1.88068059
C	-2.99716987	0.34610161	2.27675278
C	-3.53569700	-0.43815975	1.08249728
H	-3.28413409	-1.49818889	1.14936590
H	-1.78955923	1.98028653	0.17886842
H	-1.08081217	1.44384249	2.41927895
H	-3.54310699	1.28386475	2.37878580
H	-4.61096298	-0.33505361	0.96130816
H	-0.94023939	-0.27302704	2.03020587
H	-3.07958877	-0.20822519	3.20766865
N	0.61794436	1.27319550	-0.44932883
C	1.92220447	0.78413567	-0.89607035
C	2.33671985	-0.42898890	-0.08154869
O	2.13007671	-0.41722635	1.16352778

C	2.84978250	1.98195507	-0.64134115
C	1.92198863	3.17803144	-0.85875159
C	0.60331819	2.73124646	-0.22842353
H	0.57459810	2.94219656	0.83944820
H	1.87189168	0.54305080	-1.95439361
H	3.71166445	1.97133980	-1.30240142
H	1.78135810	3.35237698	-1.92489141
H	-0.25805004	3.17809560	-0.71714768
H	3.19662636	1.95927077	0.39205752
H	2.30082051	4.08959862	-0.40560685
N	2.94944168	-1.43285337	-0.67195136
C	3.41116603	-2.57648787	0.11426094
H	4.35659919	-2.91856637	-0.29644837
H	2.68021903	-3.38287760	0.06315234
H	3.55153132	-2.27802843	1.14639967
C	3.07676629	-1.53398613	-2.12993068
H	2.09451258	-1.59466102	-2.59426967
H	3.62412460	-2.44296546	-2.35270253
H	3.63100999	-0.69058892	-2.53337290
F	1.00484914	-2.38300804	2.25883783
H	1.44949309	-1.64741077	1.84245146
F	1.56564343	1.58540519	2.50611097
H	1.76282606	0.82093972	1.95008855
H	-4.30459892	-1.69012501	-1.25837322
H	-4.46892053	-0.76137743	-2.77005596
F	-1.86214006	-2.61157376	-0.57442097
H	-1.26591646	-1.84042291	-0.57105340

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Ac-Pro2-NMe2-trans-xx

M062X/6311pp2d2p/H2O optimized

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C	4.13083876	0.51434263	2.09014962
C	2.98966987	0.71673716	1.12595042
O	2.23576430	1.68858661	1.19120848
H	5.08337397	0.64606175	1.57633419
N	2.82671892	-0.21824538	0.17335512
C	1.73398020	-0.09972276	-0.78526212
C	0.38831572	-0.05884508	-0.06807924
O	0.13211510	-0.87577808	0.81273074
C	1.85940305	-1.38006444	-1.62844701
C	3.34350466	-1.73792589	-1.51496872
C	3.66279489	-1.39675719	-0.06199049
H	3.37192754	-2.21067548	0.60641693
H	1.88151369	0.78787341	-1.39701510
H	1.52385988	-1.22494879	-2.65035508
H	3.93688743	-1.10782967	-2.17761300
H	4.71281503	-1.16763521	0.10032469
H	1.25366373	-2.16441607	-1.17434805
H	3.54659006	-2.77935389	-1.75049281
N	-0.52337701	0.82936929	-0.49137086
C	-1.86520242	0.78247283	0.07529655
C	-2.52427759	-0.56876952	-0.21188960
O	-2.24901748	-1.17769275	-1.24029475
C	-2.59903210	1.92072965	-0.65007921
C	-1.47829403	2.90934269	-0.97090774
C	-0.31225102	1.99956394	-1.35249000
H	-0.35857134	1.71573339	-2.40566420
H	-1.80219127	0.96439449	1.14690265
H	-3.39544276	2.34728328	-0.04566517
H	-1.21856321	3.48249074	-0.08081912
H	0.65131380	2.45632707	-1.14431579
H	-3.03109265	1.53504373	-1.57454625
H	-1.73768201	3.60226588	-1.76688324
N	-3.44593853	-0.99438125	0.67494453
C	-4.09139137	-2.28463708	0.48995835
H	-5.17276421	-2.15682017	0.44571078
H	-3.85097141	-2.94234120	1.32625574
H	-3.73937366	-2.72895552	-0.43306251
C	-3.76581379	-0.29180972	1.91193201
H	-3.01226525	-0.46734656	2.68126068
H	-4.72004189	-0.66660445	2.27298751
H	-3.87348902	0.77678140	1.74767373
H	4.11466690	-0.49099345	2.50887848
H	4.04964863	1.24759734	2.88534074

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Ac-Pro2-NMe2-trans-xx-P2HFHF

M062X/6311pp2d2p/H2O optimized

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C	4.42055601	-0.94786981	-1.91707204
C	3.23244497	-0.97040037	-0.98987836
O	2.53631126	-1.97457642	-0.83283645
H	5.34267378	-0.90805491	-1.33625326
N	2.95946075	0.16460746	-0.32260716
C	1.83390007	0.20884430	0.60384948
C	0.53144477	-0.14238741	-0.10293504
O	0.20877453	0.41726588	-1.14723817
C	1.82071688	1.67019282	1.07860111
C	3.28566146	2.09334753	0.94841825
C	3.72306679	1.41527747	-0.34739174
H	3.44680136	2.01258911	-1.21914188
H	2.01708304	-0.47100842	1.43403127
H	1.41926895	1.76119065	2.08344616
H	3.86732988	1.70004381	1.78223940
H	4.79103086	1.21559114	-0.38323120
H	1.20241448	2.25749239	0.39912698
H	3.41371844	3.17201823	0.91395367
N	-0.29604555	-1.00608981	0.51020667
C	-1.61217357	-1.24195162	-0.06300337
C	-2.36398635	0.06463570	-0.23245860
O	-2.20419205	0.97762323	0.62219259
C	-2.28875051	-2.15052164	0.97521416
C	-1.11069011	-2.95594640	1.52451506
C	0.01359133	-1.92347295	1.61747953

H	-0.01288203	-1.38682410	2.56553389
H	-1.50890242	-1.74347072	-1.02324129
H	-3.07216834	-2.76164845	0.53515442
H	-0.83669249	-3.73958007	0.81847597
H	0.99480966	-2.36746391	1.47033005
H	-2.72408460	-1.53476999	1.76393956
H	-1.32574415	-3.41523793	2.48534918
N	-3.22077279	0.19159236	-1.22653189
C	-4.00530291	1.41752437	-1.36904588
H	-4.98436576	1.15607778	-1.75892890
H	-3.51237007	2.10420492	-2.05631523
H	-4.11769044	1.89338983	-0.40141048
C	-3.35224374	-0.81380814	-2.28585136
H	-2.45887948	-0.83702029	-2.90738938
H	-4.20083015	-0.53846206	-2.90203303
H	-3.53912139	-1.79871540	-1.86679210
F	-1.80049521	3.34245339	-0.09648513
H	-1.97080653	2.43830549	0.16888135
F	-0.95833184	0.84937978	2.77278748
H	-1.40917815	0.83788055	1.92106516
H	4.39793509	-0.07369533	-2.56611962
H	4.41503649	-1.85338543	-2.51445629

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