Supplementary Information – HyDRA challenge

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1 Computational Details

We used two composite schemes developed over the last decade to investigate the spectroscopy and the dynamics of weakly bound molecular systems. The first scheme combines the use of the PBE0 functional [DOI:10.1063/1.478522], Grimme's D3 dispersion correction [DOI:10.1063/1.3382344] and the explicitly correlated coupled cluster method (CCSD-F12)) technique [DOI:10.1063/1.2817618, DOI:10.1063/1.3054300] the second one combines the use of the PBE0 functional, Grimme's D3 dispersion correction and the explicitly correlated Möller-Plesset method (MP2-F12) [DOI:10.1063/1.2889388]

First, full geometry optimizations were performed for all complexes. These computations were carried out in the C_1 point group at the PBE0-D3/aug-cc-pVTZ level [DOI:10.1063/1.456153, DOI:10.1063/1.464303, DOI:10.1063/1.462569] as implemented in the Gaussian16 program package [https://gaussian.com/citation/]. Harmonic and anharmonic frequency calculations were carried out to check the nature of the stationary points (minimum or transition state) and to evaluate the zero-point vibrational energy (ZPE) corrections of the considered molecular clusters. geometry optimizations and harmonic frequency computations using the CCSD-F12 and MP2-F12 methods were then performed whereby the aug-cc-pVDZ basis set was used in conjunction with the corresponding resolutions of the identity and density fitting functions as generated by MOLPRO (Version 2019.2)[https://www.molpro.net.].

The PBE0-D3/aug-cc-pVTZ//MP2-F12/aug-cc-pVDZ or PBE0-D3/aug-cc-pVTZ//CCSD-F12/aug-cc-pVDZ composite schemes where then used to determine the OH stretching wavenumber frequencies (ν_i). Here, ν_i is equal to $\omega_i + \Delta\nu_i$, where ω_i is the harmonic frequency at the MP2-F12/aug-cc-pVDZ or the CCSD-F12/aug-cc-pVDZ depending on the composite sheme used and $\Delta\nu_i$ is the corresponding PBE0-D3/aug-cc-pVTZ anharmonic correction ($\Delta\nu_i = \nu_{i,PBE0} - \omega_{i,PBE0}$ at the PBE0-D3/aug-cc-pVTZ level of theory).

2 Additional computed data (optional)

2.1 OH-stretching fundamentals for test set

OH stretching fundamentals computed using the PBE0-D3/aug-cc-pVTZ//CCSD-F12/aug-cc-pVDZ (anharmonic frequencies) composite scheme.

Code	CAS	fundamentals (cm^{-1})	description
H_2O	----	3793	v(OH)as
			v(OH)s
		3700	reference
			value

CON(S1)	502-49-8	---	---
		---	---
CON(S2)	502-49-8	---	---
		---	---
CON(S3)	502-49-8	---	---
		---	---
DMI(S1)	80-73-9	---	---
		---	---
DMI(S2)	80-73-9	---	---
		---	---
FAH	50-0-0	3760	v(OH)
		3654	v(OH)
MLA	547-64-8	---	---
		---	---
		---	---
PCD	125132-75-4	---	---
		---	---
		---	---
		---	---
PYR	110-86-1	3763	v(OH)
		3527	v(OH)
THF(S1)	109-99-9	3771	v(OH)
		3587	v(OH)
THF(S2)	109-99-9		---

THT	110-01-0	3772	v(OH)
		3571	v(OH)
TPH(S1)	434-45-7	---	---
		---	---
TPH(S2)	434-45-7	---	---
		---	---
TPH(S3)	434-45-7	---	---
		---	---
TFE(S1)	75-89-8	---	---
		---	---
		---	---
TFE(S2)	75-89-8	---	---
		---	---

		---	---
TFE(S3)	75-89-8	---	---
		---	---
		---	---
TFE(S4)	75-89-8	---	---
		---	---
		---	---
TFE(S5)	75-89-8	---	---
		---	---
		---	---

OH stretching fundamentals computed using the PBE0-D3/aug-cc-pVTZ//MP2-F12/aug-cc-pVDZ (anharmonic frequencies) composite scheme.

Code	CAS	fundamentals (cm^{-1})	description
H_2O	----	3785	v(OH)as
			v(OH)s
		3672	reference value
CON(S1)	502-49-8	---	---
		---	---
CON(S2)	502-49-8	---	---
		---	---
CON(S3)	502-49-8	---	---
		---	---
DMI(S1)	80-73-9	---	---
		---	---
DMI(S2)	80-73-9	---	---
		---	---
FAH	50-0-0	3741	v(OH)
		3582	v(OH)
MLA	547-64-8	---	---
		---	---
		---	---
PCD	125132-75-4	---	---
		---	---
		---	---
		---	---

PYR	110-86-1	3746	v(OH)
		3405	v(OH)
THF(S1)	109-99-9	3751	v(OH)
		3479	v(OH)
THF(S2)	109-99-9		---

THT	110-01-0	3750	v(OH)
		3474	v(OH)
TPH(S1)	434-45-7	---	---
		---	---
TPH(S2)	434-45-7	---	---
		---	---
TPH(S3)	434-45-7	---	---
		---	---
TFE(S1)	75-89-8	3773	v(OH)
		3659	v(OH)
		3499	v(OH)
TFE(S2)	75-89-8	---	---
		---	---
		---	---
TFE(S3)	75-89-8	---	---
		---	---
		---	---
TFE(S4)	75-89-8	3769	v(OH)
		3679	v(OH)
		3656	v(OH)
TFE(S5)	75-89-8	---	---
		---	---
		---	---

OH stretching fundamentals (Harmonic and anharmonic frequencies) computed at the PBE0-D3/aug-cc-pVTZ level of theory.

Code	CAS	Harmonic (cm^{-1})	Anharmonic (cm^{-1})	description
H_2O	----	3965	3784	v(OH)as
				v(OH)s
		3859	3691	reference
				value
CON(S1)	502-49-8	3929	---	v(OH)

		3621	---	v(OH)
CON(S2)	502-49-8	3929	---	v(OH)
		3634	---	v(OH)
CON(S3)	502-49-8	3954	---	v(OH)
		3848	---	v(OH)
DMI(S1)	80-73-9	3930	---	v(OH)
		3611	---	v(OH)
DMI(S2)	80-73-9	3931	---	v(OH)
		3615	---	v(OH)
FAH	50-0-0	3937	3745	v(OH)
		3731	3588	v(OH)
MLA	547-64-8	3922	---	v(OH)
		3636	---	v(OH)
		3571	---	v(OH)
PCD	125132-75-4	---	---	---
		---	---	---
		---	---	---
		---	---	---
PYR	110-86-1	3925	3752	v(OH)
		3548	3398	v(OH)
THF(S1)	109-99-9	3929	3759	v(OH)
		3629	3501	v(OH)
THF(S2)	109-99-9	3956	---	v(OH)
		3852	---	v(OH)
THT	110-01-0	3921	3755	v(OH)
		3631	3455	v(OH)
TPH(S1)	434-45-7	3935	---	v(OH)
		3790	---	v(OH)
TPH(S2)	434-45-7	3950	---	v(OH)
		3850	---	v(OH)
TPH(S3)	434-45-7	3942	---	v(OH)
		3845	---	v(OH)
TFE(S1)	75-89-8	3947	3772	v(OH)
		3843	3679	v(OH)
		3624	3455	v(OH)
TFE(S2)	75-89-8	3954	3776	v(OH)
		3848	3682	v(OH)
		3642	3502	v(OH)

TFE(S3)	75-89-8	3934	3760	v(OH)
		3865	3707	v(OH)
		3767	3612	v(OH)
TFE(S4)	75-89-8	3955	3768	v(OH)
		3864	3697	v(OH)
		3851	3676	v(OH)
TFE(S5)	75-89-8	3934	3757	v(OH)
		3865	3681	v(OH)
		3767	3607	v(OH)

OH stretching fundamentals computed at the CCSD-F12/aug-cc-pVDZ (harmonic frequencies) level of theory.

Code	CAS	fundamentals (cm^{-1})	description
H_2O	----	3974	v(OH)as
			v(OH)s
		3868	reference
			value
CON(S1)	502-49-8	---	---
		---	---
CON(S2)	502-49-8	---	---
		---	---
CON(S3)	502-49-8	---	---
		---	---
DMI(S1)	80-73-9	---	---
		---	---
DMI(S2)	80-73-9	---	---
		---	---
FAH	50-0-0	3952	v(OH)
		3797	v(OH)
MLA	547-64-8	---	---
		---	---
		---	---
PCD	125132-75-4	---	---
		---	---
		---	---

		---	---
PYR	110-86-1	3937	v(OH)
		3677	v(OH)
THF(S1)	109-99-9	3941	v(OH)
		3715	v(OH)
THF(S2)	109-99-9	3964	---
		3857	---
THT	110-01-0	3937	v(OH)
		3747	v(OH)
TPH(S1)	434-45-7	---	---
		---	---
TPH(S2)	434-45-7	---	---
		---	---
TPH(S3)	434-45-7	---	---
		---	---
TFE(S1)	75-89-8	---	---
		---	---

TFE(S2)	75-89-8	---	---
		---	---
		---	---
TFE(S3)	75-89-8	---	---
		---	---
		---	---
TFE(S4)	75-89-8	---	---
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TFE(S5)	75-89-8	---	---
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		---	---

OH stretching fundamentals computed at the MP2-F12/aug-cc-pVDZ (harmonic frequencies) level of theory.

Code	CAS	fundamentals (cm^{-1})	description
H_2O	----	3966	v(OH)as

		3840	v(OH)s reference value
CON(S1)	502-49-8	--- ---	--- ---
CON(S2)	502-49-8	--- ---	--- ---
CON(S3)	502-49-8	--- ---	--- ---
DMI(S1)	80-73-9	--- ---	--- ---
DMI(S2)	80-73-9	--- ---	--- ---
FAH	50-0-0	3933 3726	v(OH) v(OH)
MLA	547-64-8	--- --- ---	--- --- ---
PCD	125132-75-4	--- --- --- ---	--- --- --- ---
PYR	110-86-1	3919 3555	v(OH) v(OH)
THF(S1)	109-99-9	3921 3607	v(OH) v(OH)
THF(S2)	109-99-9		--- ---
THT	110-01-0	3915 3651	v(OH) v(OH)
TPH(S1)	434-45-7	--- ---	--- ---
TPH(S2)	434-45-7	--- ---	--- ---
TPH(S3)	434-45-7	--- ---	--- ---
TFE(S1)	75-89-8	3947 3822	v(OH) v(OH)

		3668	v(OH)
TFE(S2)	75-89-8	---	---
		---	---
		---	---
TFE(S3)	75-89-8	---	---
		---	---
		---	---
TFE(S4)	75-89-8	3956	---
		3846	---
		3831	---
TFE(S5)	75-89-8	---	---
		---	---
		---	---

2.2 IR intensities and Raman scattering activities

IR intensities computed at the PBE0-D3/aug-cc-pVTZ level of theory.

Code	CAS	IR intensities ($km.mol^{-1}$)
H_2O	----	67.0
		5.6
CON(S1)	502-49-8	81.2
		558.8
CON(S2)	502-49-8	83.0
		527.4
CON(S3)	502-49-8	117.1
		12.0
DMI(S1)	80-73-9	81.5
		698.5
DMI(S2)	80-73-9	97.9
		702.2
FAH	50-0-0	96.2
		251.4
MLA	547-64-8	92.4
		759.0
		138.7
PCD	125132-75-4	---

PYR	110-86-1	73.6
		979.9
THF(S1)	109-99-9	83.6
		569.7
THF(S2)	109-99-9	69.8
		4.4
THT	110-01-0	88.3
		458.7
TPH(S1)	434-45-7	137.1
		369.7
TPH(S2)	434-45-7	75.9
		10.9
TPH(S3)	434-45-7	75.1
		35.7
TFE(S1)	75-89-8	106.6
		14.2
		603.9
TFE(S2)	75-89-8	104.2
		14.4
		572.1
TFE(S3)	75-89-8	108.5
		61.2
		216.3
TFE(S4)	75-89-8	82.7
		50.0
		9.0
TFE(S5)	75-89-8	108.5
		61.2
		216.6

2.3 Isotopolog information

No further information has been made available.

2.4 Relative energies for local minima and spectral properties

Relative energies of CON (502-49-8) computed at the PBE0-D3/aug-cc-pVTZ level of theory.

Method	CON 502-49-8	S1	S2	S3
PBE0-D3/aug-cc-pVTZ	E (kJ/mol)	0	1.303	25.837

Relative energies of DMI (80-73-9) computed at the PBE0-D3/aug-cc-pVTZ level of theory.

Method	DMI 80-73-9	S1	S2
PBE0-D3/aug-cc-pVTZ	E (kJ/mol)	0	0.089

Relative energies of THF (109-99-9) computed at different levels of theories.

Method	THF 109-99-9	S1	S2
PBE0-D3/aug-cc-pVTZ	E (kJ/mol)	0	21.415
MP2-F12/aug-cc-pVDZ	E (kJ/mol)	0	21.670
CCSD-F12/aug-cc-pVDZ	E (kJ/mol)	0	19.350

Relative energies of TPH (434-45-7) computed at the PBE0-D3/aug-cc-pVTZ level of theory.

Method	TPH 434-45-7	S1	S2	S3
PBE0-D3/aug-cc-pVTZ	E (kJ/mol)	0	4.019	6.938

Relative energies of THE (75-89-8) computed at different levels of theories.

Method	TFE 75-89-8	S1	S2	S3	S4	S5
PBE0-D3/aug-cc-pVTZ	E (kJ/mol)	0	1.668	12.459	18.655	19.454
MP2-F12/aug-cc-pVDZ	E (kJ/mol)	0	---	---	17.900	---

2.5 Other computed quantities for the training and test sets

Structures optimized at the PBE0-D3/aug-cc-pVTZ level of theory.

Code	CAS	XYZ (Ångström)
H_2O	----	O 0.00000000 0.00000000 0.11687400 H 0.00000000 0.75994600 -0.46749600 H 0.00000000 -0.75994600 -0.46749600
CON(S1)	502-49-8	C 0.63346400 1.06160400 0.28012100 C -0.57628400 1.94698500 0.40747700 C -1.13386400 -1.81078600 0.43544700

		C -1.87456300 1.15657900 0.22451700
		C -1.97988600 -1.24805800 -0.70743300
		C -1.82785700 0.24153600 -1.00907100
		H -0.48665000 2.73268900 -0.34409900
		H -2.07142500 0.56628100 1.12229600
		H -1.56485400 -1.51770600 1.39892600
		H -3.02935900 -1.46544000 -0.48183100
		H -0.55614200 2.41741000 1.39697200
		H -1.23632000 -2.89917100 0.40054300
		H -2.69934500 1.86778600 0.15362300
		H -1.74909900 -1.80208100 -1.62276000
		H -2.60387900 0.52833400 -1.72251100
		H -0.88399100 0.39920100 -1.53990900
		C 0.74110200 -0.15786500 1.15782600
		H 0.13700300 -0.03844500 2.06085100
		H 1.79070500 -0.22836800 1.44983200
		C 0.35644300 -1.47167600 0.44715600
		H 0.77333300 -1.46940300 -0.56375000
		H 0.88297700 -2.26817700 0.97594900
		O 1.49778300 1.30698800 -0.53940800
		O 3.50878800 -0.66047900 -0.52398300
		H 4.31489500 -0.39388800 -0.96674100
		H 2.89825300 0.08898100 -0.62651000
CON(S2)	502-49-8	C 0.65669100 -1.01418600 0.41520200
		C 0.92745100 0.10595800 1.38091600
		C -2.43937100 0.03289700 -0.36269000
		C -0.11956300 1.21799600 1.25570900
		C -1.79558900 1.37774900 -0.70264500
		C -0.37031200 1.61782500 -0.20637800
		H 1.92642200 0.49419200 1.18028700
		H -1.05325300 0.89963900 1.72563300
		H -2.73349800 0.01523200 0.69222200
		H -2.45080000 2.16151500 -0.30771700
		H 0.91636000 -0.30875300 2.39527700
		H -3.37999900 -0.01837700 -0.91859200
		H 0.22809400 2.07192400 1.83918000
		H -1.79982300 1.50520600 -1.78983600
		H -0.13080900 2.67285600 -0.35439500
		H 0.33188100 1.08367800 -0.85281700
		C -0.68402400 -1.70167900 0.45440000
		H -1.16368900 -1.57219300 1.42776400

		H -0.47718200 -2.76434800 0.31266600
		C -1.63922700 -1.23536200 -0.66121100
		H -1.07575800 -1.13377900 -1.59366700
		H -2.34839400 -2.04996500 -0.82425200
		O 1.47447300 -1.35454100 -0.41749200
		O 3.40191000 0.64227900 -0.85530900
		H 4.13659500 0.38488300 -1.41290200
		H 2.84645500 -0.15080300 -0.77626800
CON(S3)	502-49-8	C 2.09726300 -0.44489600 -0.15747900
		C 2.27367500 0.95026500 0.39055600
		C -1.20549100 -0.56453600 0.54633600
		C 0.92870800 1.63665700 0.64033800
		C -1.32323700 0.73953900 -0.24375300
		C -0.02740700 1.48810900 -0.55307300
		H 2.86813300 1.50859500 -0.33427200
		H 0.46973400 1.22373900 1.54156800
		H -1.00708400 -0.34206700 1.59997300
		H -1.99255000 1.40389400 0.31610400
		H 2.84473900 0.88861500 1.32369800
		H -2.19313100 -1.03238000 0.53674900
		H 1.11548400 2.68902000 0.86172500
		H -1.81792200 0.52773700 -1.19928100
		H -0.28529600 2.46982000 -0.95739100
		H 0.49072900 0.97252200 -1.36707000
		C 1.24894700 -1.42462100 0.62186200
		H 1.19957800 -1.14900300 1.67889800
		H 1.76403900 -2.38403500 0.54418300
		C -0.17778800 -1.58915200 0.06510900
		H -0.13315400 -1.61753300 -1.02807300
		H -0.52379600 -2.57726100 0.37630900
		O 2.59158900 -0.77471800 -1.21100300
		O -4.62445600 -0.19154500 -0.12176700
		H -3.99704900 0.44828500 -0.46489800
		H -5.42753800 -0.04803800 -0.62543800
DMI(S1)	80-73-9	O 0.88550500 -1.09552900 0.30439700
		N 0.06428100 1.03253500 -0.10688500
		N -1.36886000 -0.63783300 0.17643200
		C -1.23761000 1.65286700 -0.03084600
		C -2.16784300 0.47165100 -0.28633200
		C -0.03566000 -0.31003400 0.14081800
		C 1.25181100 1.78399500 0.19696800

		C -1.80002100 -1.99350000 -0.01394500
		H -1.34764500 2.44620600 -0.77177500
		H -1.40591500 2.08430200 0.96600400
		H -3.10881100 0.54829200 0.26076600
		H -2.39632000 0.36866300 -1.35668500
		H 2.12538300 1.14095000 0.11015700
		H 1.21435600 2.19797500 1.21272300
		H 1.35594100 2.60891200 -0.51008400
		H -0.99824000 -2.65590200 0.30721500
		H -2.02900100 -2.20147900 -1.06705600
		H -2.69159900 -2.19474700 0.58290300
		O 3.56382400 -0.71748400 -0.34734300
		H 2.64682200 -0.94433100 -0.11341600
		H 4.10838600 -1.28751800 0.19600200
DMI(S2)	80-73-9	O 0.88672500 -1.11307000 0.03666200
		N 0.03973700 1.03483600 -0.17559900
		N -1.36372100 -0.64523000 0.18527500
		C -1.23990300 1.65188900 0.08472100
		C -2.20200900 0.48747800 -0.12582100
		C -0.04057000 -0.31844100 0.01727500
		C 1.26049300 1.76811900 0.02406200
		C -1.82418000 -1.98982400 -0.01186800
		H -1.42838700 2.48506400 -0.59405100
		H -1.28926100 2.02746000 1.11647900
		H -3.07440700 0.53618100 0.52774600
		H -2.55097700 0.44193500 -1.16738800
		H 2.11281400 1.13645600 -0.21753500
		H 1.36037000 2.10930800 1.06202300
		H 1.27405600 2.64097800 -0.63114900
		H -0.99660200 -2.66769300 0.18926000
		H -2.17233300 -2.15259400 -1.04008600
		H -2.64434900 -2.21353200 0.67292700
		O 3.63839700 -0.68575800 0.03248000
		H 2.69521600 -0.92453900 0.04428900
		H 4.05779600 -1.35097400 -0.51358500
FAH	50-0-0	C -1.30100600 0.46100200 -0.00005700
		H -0.60041500 1.31452100 -0.00030100
		H -2.38127700 0.69377100 0.00009000
		O -0.90761000 -0.67451300 0.00002800
		O 1.80329900 0.17858500 0.00016900
		H 1.04522100 -0.42130100 0.00000200

		H 2.57700200 -0.38557700 -0.00102900
MLA	547-64-8	O 1.51868800 0.68841600 -1.09733000 C 0.39645700 1.08330800 -0.37140100 C -0.59128300 -0.05811100 -0.18207200 O -0.29636000 -1.22331500 -0.04155900 O -1.84579700 0.37892200 -0.13754200 C -2.84143800 -0.61096400 0.12558200 C 0.74554000 1.64772900 1.00305100 H 2.00561400 0.01325200 -0.59258700 H -0.10878400 1.85123400 -0.96141800 H -3.78972800 -0.08061600 0.13652800 H -2.83631000 -1.37127500 -0.65521700 H -2.65768700 -1.08922800 1.08783800 H 1.42234500 2.49242700 0.87531100 H 1.24898200 0.88798600 1.60472800 H -0.14700500 1.98578700 1.53256500 O 2.40636700 -1.49275600 0.43188700 H 1.46103700 -1.67499500 0.28866600 H 2.88269600 -2.19647400 -0.01102300
PCD	125132-75-4	---
PYR	110-86-1	C -0.08902500 -1.13990600 0.01971200 C -1.47406700 -1.19219500 -0.00558500 C -2.17989100 0.00011400 -0.01799000 C -1.47387100 1.19230400 -0.00555400 C -0.08883300 1.13978500 0.01973600 N 0.59558100 -0.00011500 0.03360500 H -3.26308800 0.00020400 -0.03837400 H 0.50108900 -2.05057900 0.02675600 H -1.98255300 -2.14764900 -0.01660700 H -1.98219800 2.14784300 -0.01654400 H 0.50142100 2.05036700 0.02678000 O 3.45278100 0.00007400 -0.12666600 H 2.48073800 -0.00003900 -0.03641400 H 3.78740200 -0.00054700 0.77058100
THF(S1)	109-99-9	C -0.44795200 -1.22292000 0.19379900 O 0.29375700 -0.19549900 0.86330100 C -0.32135800 1.07098100 0.62816300 C -1.14217600 0.89007300 -0.63313700 C -1.64355200 -0.53924300 -0.45806800 H 0.20843800 -1.68536700 -0.54968200 H -0.73628800 -1.98222600 0.92426300

		H -0.95728600 1.33262700 1.48293100
		H 0.46968700 1.81668900 0.53694900
		H -1.94409500 1.62259500 -0.72550500
		H -0.49697000 0.96720700 -1.51127700
		H -2.50743100 -0.55648100 0.21076700
		H -1.93190900 -1.01598400 -1.39467300
		O 2.68287500 0.01566000 -0.53978300
		H 3.47183800 -0.15203800 -0.02373000
		H 1.94119100 -0.10165500 0.07727500
THF(S2)	109-99-9	C -0.74773500 -1.12450000 -0.40559000
		O -1.44541900 0.00031800 -0.90046700
		C -0.74734500 1.12471800 -0.40522400
		C -0.33884000 0.77024200 1.02578200
		C -0.33912700 -0.77063500 1.02552700
		H -1.40679500 -1.98974300 -0.48048100
		H 0.14277700 -1.31656700 -1.02391000
		H 0.14324700 1.31668800 -1.02345600
		H -1.40609700 1.99022400 -0.47980400
		H 0.63961900 1.17955500 1.27413800
		H -1.06457100 1.15969100 1.74032200
		H 0.63917000 -1.18039700 1.27379700
		H -1.06502400 -1.16004900 1.73991700
		O 2.74022900 -0.00001000 -0.22436200
		H 2.36746700 -0.00067500 -1.10821800
		H 3.69000700 -0.00014300 -0.35664300
THT	110-01-0	C -0.44419300 0.09153900 -1.37852700
		S 0.05688000 -1.26314600 -0.25310900
		C -0.60498500 -0.43797700 1.24444700
		C -1.47221000 0.70564200 0.74086600
		C -0.76877900 1.27534100 -0.48148600
		H 0.37530100 0.29695500 -2.06614500
		H -1.31454800 -0.23143100 -1.95148700
		H -1.16112000 -1.16751000 1.83160300
		H 0.23269500 -0.06794100 1.83663600
		H -2.45826900 0.32559100 0.45847200
		H -1.61524900 1.45678000 1.52086600
		H -1.38556400 2.00696000 -1.00857100
		H 0.15906300 1.76740100 -0.17940700
		O 2.56455900 0.71096000 0.30904000
		H 3.46753500 0.39150100 0.28063100
		H 2.01461100 -0.06291600 0.10303300

		C	-2.849417	-1.848990	0.000000
		C	-2.189560	-3.072602	0.000000
		C	-0.803031	-3.119323	0.000000
		C	-0.068103	-1.946067	0.000000
		C	-0.725357	-0.714316	0.000000
		C	-2.122282	-0.675391	0.000000
		H	-3.931601	-1.814859	0.000000
		H	-2.760039	-3.993607	0.000000
		H	-0.291281	-4.073368	0.000000
		H	1.011480	-1.998506	0.000000
TPH(S1)	434-45-7	H	-2.614991	0.288500	0.000000
		C	-0.019297	0.577689	0.000000
		O	-0.576687	1.646583	0.000000
		C	1.535238	0.575368	0.000000
		F	2.010031	-0.051926	1.082755
		F	2.010031	-0.051926	-1.082755
		F	2.010031	1.810507	0.000000
		O	0.162474	4.530284	0.000000
		H	1.119550	4.571023	0.000000
		H	-0.039407	3.587769	0.000000
		C	-3.291597	-0.648578	-0.035749
		C	-3.348533	0.740038	0.017671
		C	-2.179713	1.484700	0.063948
		C	-0.947219	0.851551	0.057755
		C	-0.885616	-0.541762	0.002643
		C	-2.067450	-1.286583	-0.043737
		H	-4.204913	-1.229310	-0.072030
		H	-4.309248	1.241108	0.022471
		H	-2.220338	2.565958	0.103474
		H	-0.054459	1.461179	0.095357
TPH(S2)	434-45-7	H	-1.998608	-2.366144	-0.086383
		C	0.380179	-1.299078	-0.013095
		O	0.452487	-2.499147	-0.055103
		C	1.720301	-0.508644	0.025888
		F	1.824726	0.314540	-1.034190
		F	1.808801	0.242713	1.132043
		F	2.756714	-1.325638	0.003295
		O	1.432940	3.294527	-0.125665
		H	1.972471	2.706249	-0.658846
		H	1.937400	3.423527	0.679816
TPH(S3)	434-45-7	C	2.852908	-1.087638	-0.387724

		C	3.216570	-0.171418	0.592082
		C	2.241607	0.524880	1.292994
		C	0.900663	0.316034	1.012457
		C	0.530819	-0.600227	0.025964
		C	1.517375	-1.304110	-0.667113
		H	3.614485	-1.627695	-0.935910
		H	4.263674	0.001746	0.808738
		H	2.525314	1.236460	2.057998
		H	0.153177	0.868310	1.564712
		H	1.211333	-2.008520	-1.429963
		C	-0.873429	-0.867540	-0.351358
		O	-1.214756	-1.742556	-1.100337
		C	-1.978645	0.056233	0.234075
		F	-2.046746	-0.063281	1.566697
		F	-1.713165	1.345643	-0.045085
		F	-3.161614	-0.234630	-0.268458
		O	1.030482	2.552590	-1.586403
		H	1.453459	1.925192	-0.995675
		H	0.099286	2.497362	-1.362635
TFE(S1)	75-89-8	F 1.39925600 0.13817700 1.19300300 F 1.88910000 -0.49957600 -0.81198700 F 0.08234500 -1.20845700 0.14429000 O -0.91616700 1.47050900 0.20622900 C 0.13233700 1.04653800 -0.59888200 C 0.88467600 -0.12982800 -0.00635700 H 0.85223500 1.86144700 -0.69786500 H -0.18415600 0.74471400 -1.60466100 H -1.65152000 0.84197200 0.11524600 O -2.78941000 -0.57887000 -0.13329200 H -2.24820700 -1.32280400 0.14402300 H -3.59363000 -0.63062100 0.38676200			
TFE(S2)	75-89-8	F 1.42239000 0.16424300 1.17086900 F 1.87238700 -0.51779300 -0.82907400 F 0.08676000 -1.20696000 0.17922600 O -0.90952700 1.48291000 0.19681800 C 0.12007300 1.03165600 -0.61590400 C 0.88396500 -0.13102400 -0.01026800 H 0.84003500 1.84111800 -0.75247300 H -0.21557700 0.70380200 -1.60778800 H -1.64721500 0.85314900 0.14964900 O -2.80676900 -0.56568400 0.03291000			

		H -2.25447000 -1.34899500 0.09484200
		H -3.45045600 -0.74608600 -0.65421500
TFE(S3)	75-89-8	F -0.97140600 0.55455300 -1.26377800 F -1.75331800 1.02631800 0.69489100 F -1.73844600 -1.02289400 -0.00848200 O 1.05915800 -1.04628300 -0.05346800 C 0.31742000 -0.06761300 0.62522000 C -1.04570600 0.13119200 -0.00206900 H 0.87235500 0.86789000 0.55699400 H 0.16282300 -0.30961900 1.68128000 H 0.64812900 -1.90505300 0.06983300 O 3.44997500 0.48894200 0.05808100 H 2.87098800 -0.25346600 -0.15113600 H 3.93630400 0.66702900 -0.74782800
TFE(S4)	75-89-8	F 0.16205000 0.58160300 1.29409500 F -0.47165500 1.21722000 -0.67129900 F 1.63536600 0.99520500 -0.22429100 O 1.32358500 -1.77240700 0.14171600 C 0.36369800 -0.97514900 -0.48826100 C 0.42166200 0.45931200 -0.00780300 H -0.62492900 -1.36246200 -0.24296800 H 0.47030100 -0.95258300 -1.57887200 H 2.19856500 -1.47350100 -0.11709100 O -2.90032800 -0.49725100 -0.05093700 H -3.44155100 -0.52587900 0.73993000 H -2.63244700 0.42046300 -0.13737400
TFE(S5)	75-89-8	F -0.28616900 -1.06156500 0.74019300 F -1.65877600 -0.78859800 -0.90933800 F -1.71668600 0.54968900 0.78676000 O 0.90124500 1.36051700 0.23265800 C 0.08360300 0.74609800 -0.73390600 C -0.90234700 -0.14357700 -0.01182000 H 0.66000800 0.11103900 -1.41420200 H -0.50038100 1.46926600 -1.30990200 H 1.38034000 2.08241400 -0.17828000 O 2.97649700 -0.61994800 -0.09837400 H 2.34989700 -0.05174500 0.36519200 H 2.96593800 -1.44933700 0.38140600

Structures optimized at the CCSD-F12/aug-cc-pVDZ level of theory.

Code	CAS	XYZ (Ångström)

		O	-0.7828740803	0.6268517897	0.0000000000
H_2O	----	H	0.1734256452	0.6673901709	0.0000000000
		H	-1.0638803249	1.5418315794	0.0000000000
CON(S1)	502-49-8	---			
CON(S2)	502-49-8	---			
CON(S3)	502-49-8	---			
DMI(S1)	80-73-9	---			
DMI(S2)	80-73-9	---			
		C	-1.3031208896	0.4601204728	-0.0000312716
		H	-0.5783235025	1.2869767505	-0.0002264730
		H	-2.3721802821	0.7201787113	0.0000633156
FAH	50-0-0	O	-0.9421065750	-0.6895782581	0.0000640000
		O	1.7884781423	0.1832968535	-0.0000922616
		H	1.0594422229	-0.4457459740	-0.0000704348
		H	2.5830248840	-0.3487605559	-0.0008048746
		O	1.4904404594	0.7041329206	-1.1229809973
		C	0.3771144043	1.0994372554	-0.3775379119
		C	-0.6098626863	-0.0446882652	-0.1955015767
		O	-0.3126960788	-1.2087711428	-0.0791012043
		O	-1.8631917830	0.3950998231	-0.1260766730
		C	-2.8504153350	-0.6072588076	0.1280182294
		C	0.7526925770	1.6410673595	0.9995256905
		H	1.9852816670	0.0400652413	-0.6238358227
		H	-0.1282444921	1.8752240855	-0.9533772363
MLA	547-64-8	H	-3.7998968496	-0.0818421999	0.1568848273
		H	-2.8460866065	-1.3501144949	-0.6674045564
		H	-2.6536221603	-1.0987537965	1.0793202028
		H	1.4293929313	2.4855537359	0.8752116635
		H	1.2615546019	0.8684290036	1.5793740992
		H	-0.1319699153	1.9717237017	1.5461591294
		O	2.4228224583	-1.5006512423	0.4443761459
		H	1.5010594601	-1.7363939744	0.2745106575
		H	2.9489613475	-2.2209322031	0.0984423334
PCD	125132-75-4	---			
		C	-0.1042146187	-1.1417092245	0.0219128193
		C	-1.4916668573	-1.1936701620	-0.0065836319
		C	-2.1991015919	0.0002527451	-0.0204445724
PYR	110-86-1	C	-1.4904835710	1.1934724169	-0.0064744994
		C	-0.1030821010	1.1401447312	0.0220213805
		N	0.5854948861	-0.0011238972	0.0375362866

		H	-3.2813551286	0.0007899799	-0.0431352670
		H	0.4830569643	-2.0524772144	0.0303714173
		H	-1.9987761716	-2.1488662568	-0.0187211360
		H	-1.9966496105	2.1491692523	-0.0185260074
		H	0.4850965091	2.0503255700	0.0305673951
		O	3.5108711071	0.0012153704	-0.1270849051
		H	2.5462618338	0.0011647012	-0.0388234356
		H	3.8400343503	0.0009729879	0.7708201559
THF(S1)	109-99-9	C	-0.4589370200	-1.2311638969	0.2126770621
		O	0.2631963125	-0.2088794622	0.9128916111
		C	-0.3294220528	1.0651746750	0.6510107221
		C	-1.1119292036	0.8846954806	-0.6383766129
		C	-1.6391122414	-0.5380437134	-0.4628936353
		H	0.2143100031	-1.6808005529	-0.5217563039
		H	-0.7635781859	-1.9969511296	0.9270706954
		H	-0.9908728802	1.3356586151	1.4809355757
		H	0.4721236909	1.8000553283	0.5811056066
		H	-1.8990529219	1.6277738437	-0.7626711890
		H	-0.4353955563	0.9398119107	-1.4935908590
		H	-2.5099982962	-0.5368286430	0.1961390297
		H	-1.9182216267	-1.0183599499	-1.3998407129
		O	2.6349632829	0.0380713267	-0.5737381212
		H	3.4626374773	-0.1144929811	-0.1196241292
		H	1.9480582184	-0.1013018510	0.0922542608
THF(S2)	109-99-9	C	-0.7561635592	-1.1244781830	-0.3912584061
		O	-1.4657354985	0.0003164730	-0.8770324996
		C	-0.7558269567	1.1247405295	-0.3908844201
		C	-0.3550293422	0.7718447627	1.0455152110
		C	-0.3552388625	-0.7721767474	1.0452535311
		H	-1.4088612749	-1.9925482806	-0.4708220397
		H	0.1375051389	-1.2946709550	-1.0047288387
		H	0.1379022348	1.2948607578	-1.0042843687
		H	-1.4082637550	1.9930319422	-0.4701708016
		H	0.6210735233	1.1833424698	1.2975522866
		H	-1.0867911308	1.1595283853	1.7541580775
		H	0.6207583188	-1.1840235858	1.2971300642
		H	-1.0870895296	-1.1599026342	1.7537812988
		O	2.6806897919	-0.0003086599	-0.3962611732
		H	2.6730679819	-0.0005942521	-1.3541553760
		H	3.6095659198	-0.0002450221	-0.1624645454
THT	110-01-0	C	-0.4584020801	0.0821120985	-1.3800767114

		S	0.0185069218	-1.2816004841	-0.2596404173
		C	-0.6158101713	-0.4466990132	1.2393310953
		C	-1.4789621854	0.7089674257	0.7423521224
		C	-0.7668702368	1.2750128380	-0.4809152640
		H	0.3617266185	0.2790532157	-2.0689101819
		H	-1.3355957391	-0.2205487583	-1.9526981705
		H	-1.1756114172	-1.1656918099	1.8352893295
		H	0.2274420193	-0.0791808251	1.8244160498
		H	-2.4662929570	0.3359139372	0.4567666665
		H	-1.6132909743	1.4583805800	1.5245090897
		H	-1.3743669766	2.0135090228	-1.0076737652
		H	0.1671569494	1.7519289027	-0.1760736311
		O	2.5793764840	0.7181796039	0.3115942157
		H	3.4975382915	0.4490021983	0.2945714842
		H	2.0791824531	-0.0805899322	0.1040200881
TPH(S1)	434-45-7	---			
TPH(S2)	434-45-7	---			
TPH(S3)	434-45-7	---			
TFE(S1)	75-89-8	---			
TFE(S2)	75-89-8	---			
TFE(S3)	75-89-8	---			
TFE(S4)	75-89-8	---			
TFE(S5)	75-89-8	---			

Structures optimized at the MP2-F12/aug-cc-pVDZ level of theory.

Code	CAS	XYZ (Ångström)			
H_2O	----	O	-0.7838836010	0.6254233509	0.0000000000
		H	0.1744478276	0.6677387126	0.0000000000
		H	-1.0638929867	1.5429114765	0.0000000000
CON(S1)	502-49-8	---			
CON(S2)	502-49-8	---			
CON(S3)	502-49-8---	---			
DMI(S1)	80-73-9	---			
DMI(S2)	80-73-9	---			
FAH	50-0-0	C	-1.2877595835	0.4596424298	-0.0000268042
		H	-0.5619842791	1.2833187171	-0.0002245314
		H	-2.3553206339	0.7173579123	0.0000763404
		O	-0.9243849694	-0.6982376304	0.0000641699

		O	1.7680250064	0.1905146781	-0.0001302094
		H	1.0345412755	-0.4399648363	-0.0001150318
		H	2.5620971839	-0.3461432706	-0.0007419336
MLA	547-64-8	O	1.4901539239	0.7036668122	-1.1353218042
		C	0.3782855526	1.0953358936	-0.3795706380
		C	-0.6060544562	-0.0445868492	-0.1953428744
		O	-0.3112932185	-1.2162553849	-0.0633702677
		O	-1.8633124291	0.3999770438	-0.1366895423
		C	-2.8469911285	-0.6105386638	0.1269876829
		C	0.7602551183	1.6216478106	0.9981685588
		H	1.9889077067	0.0371272077	-0.6317173831
		H	-0.1268742907	1.8758913334	-0.9465362108
		H	-3.7959115821	-0.0888027948	0.1505521222
		H	-2.8352535307	-1.3576646364	-0.6616258515
		H	-2.6445672750	-1.0909157541	1.0805194326
		H	1.4409322763	2.4611370064	0.8781888914
		H	1.2647102407	0.8407516481	1.5667362266
		H	-0.1195923455	1.9525379917	1.5483652843
		O	2.4026938259	-1.4606152778	0.4460970774
		H	1.4741379523	-1.6924634175	0.2766650120
		H	2.9231076594	-2.1949029690	0.1139012837
PCD	125132-75-4	---			
PYR	110-86-1	C	-0.0951411387	-1.1460944652	0.0293791965
		C	-1.4829482464	-1.1938111365	-0.0075744497
		C	-2.1918810414	0.0002232089	-0.0255388678
		C	-1.4819708181	1.1936760713	-0.0074822780
		C	-0.0942028884	1.1448308105	0.0294673019
		N	0.5956762857	-0.0009144982	0.0491825082
		H	-3.2734265969	0.0006654363	-0.0544926448
		H	0.4932548309	-2.0555914227	0.0410258660
		H	-1.9911546436	-2.1482022752	-0.0227315436
		H	-1.9893971978	2.1484828912	-0.0225621204
		H	0.4949441197	2.0538403583	0.0411801405
		O	3.4738693658	0.0010421759	-0.1402823641
		H	2.5050001867	0.0008194270	-0.0285855045
		H	3.8228637826	0.0006944185	0.7524507599
THF(S1)	109-99-9	C	-0.4546867793	-1.2383087814	0.2299337602
		O	0.2557935482	-0.2198107998	0.9606157061
		C	-0.3272326388	1.0603555878	0.6732375249
		C	-1.0585082472	0.8751486325	-0.6399727221
		C	-1.6106051150	-0.5348096978	-0.4656328795

		H	0.2360249729	-1.6785837687	-0.4913198458
		H	-0.7757542131	-2.0059521032	0.9321272154
		H	-1.0167424316	1.3311198723	1.4773288337
		H	0.4803985565	1.7881717626	0.6308159877
		H	-1.8299410261	1.6250815812	-0.8024298674
		H	-0.3477888321	0.9084213317	-1.4656743118
		H	-2.4899600188	-0.5153855364	0.1783696748
		H	-1.8790984631	-1.0154946037	-1.4036806051
		O	2.5120779743	0.0578090317	-0.6152379863
		H	3.3735523416	-0.0777241141	-0.2172894508
		H	1.8712393716	-0.0956193947	0.1004019661
THF(S2)	109-99-9	C	-0.7518388470	-1.1214432344	-0.3911007628
		O	-1.4834196702	0.0003190190	-0.8632414035
		C	-0.7514994080	1.1217061726	-0.3907277284
		C	-0.3410080876	0.7706028734	1.0394680411
		C	-0.3412165001	-0.7709314975	1.0392046077
		H	-1.3954465707	-1.9940007582	-0.4706512763
		H	0.1370026543	-1.2722218433	-1.0137055363
		H	0.1373983105	1.2724122624	-1.0132675762
		H	-1.3948413651	1.9944847250	-0.4700009274
		H	0.6362764867	1.1802358255	1.2822722122
		H	-1.0674630052	1.1570970797	1.7509066715
		H	0.6359652200	-1.1809077223	1.2818425295
		H	-1.0677556136	-1.1574725970	1.7505315516
		O	2.6299918329	-0.0003259343	-0.3918391569
		H	2.6691732407	-0.0006074237	-1.3514462572
		H	3.5502443222	-0.0002299470	-0.1169169886
THT	110-01-0	C	-0.4476785993	0.0875543600	-1.3729584970
		S	0.0319001355	-1.2729643411	-0.2555696607
		C	-0.5982157063	-0.4351346855	1.2383545350
		C	-1.4724604135	0.7043525435	0.7371231561
		C	-0.7541020327	1.2761932729	-0.4745546518
		H	0.3726275378	0.2828123591	-2.0606933858
		H	-1.3249446431	-0.2165505099	-1.9425757035
		H	-1.1464756711	-1.1574377629	1.8392980805
		H	0.2448249608	-0.0549125759	1.8137814979
		H	-2.4490149653	0.3164584670	0.4403187961
		H	-1.6240112463	1.4491098598	1.5187150521
		H	-1.3552528550	2.0171809789	-1.0022391749
		H	0.1799122982	1.7451969400	-0.1623087915
		O	2.5251301029	0.7109624126	0.3057038433

		H	3.4440860977	0.4352207361	0.2894083104
		H	2.0194019997	-0.0902930545	0.0950585938
TPH(S1)	434-45-7	---			
TPH(S2)	434-45-7	---			
TPH(S3)	434-45-7	---			
TFE(S1)	75-89-8	F	1.4899860272	0.1798495829	1.1470805123
		F	1.8386717230	-0.5356854327	-0.8616303605
		F	0.0902923932	-1.1842307583	0.2363648346
		O	-0.8703056273	1.4917257841	0.2841213984
		C	0.1203895410	1.0366053370	-0.5858400094
		C	0.8935579780	-0.1251845764	-0.0041666418
		H	0.8333321560	1.8416952857	-0.7527005496
		H	-0.2726788185	0.7082919369	-1.5506352170
		H	-1.6257629603	0.8865207435	0.2148912831
		O	-2.7379632636	-0.5620081108	-0.1386487365
		H	-2.2596012514	-1.3296790746	0.1874312490
		H	-3.6430588972	-0.6746997172	0.1602412375
TFE(S2)	75-89-8	---			
TFE(S3)	75-89-8	---			
TFE(S4)	75-89-8	F	0.2844681568	0.6064779144	1.3124043500
		F	-0.4817236603	1.2080289704	-0.6165362091
		F	1.6506212084	0.9900075059	-0.3111519093
		O	1.3711948970	-1.7582416833	0.1386684566
		C	0.3638279044	-0.9773655780	-0.4489476602
		C	0.4538818975	0.4613121021	-0.0008774265
		H	-0.5987386311	-1.3655208077	-0.1288007449
		H	0.4047522731	-0.9792122994	-1.5400404658
		H	2.2233243576	-1.4642722438	-0.1964083792
		O	-2.8396744466	-0.4902420920	-0.0007505596
		H	-3.6656475629	-0.5696836354	0.4810705335
		H	-2.6619693939	0.4532828468	-0.0317849857
TFE(S5)	75-89-8	---			