Supplementary Materials: Computational Structures and SAPT Interaction Energies of $HXeYH\cdots H_2Y$ (Y=O or S) Complexes

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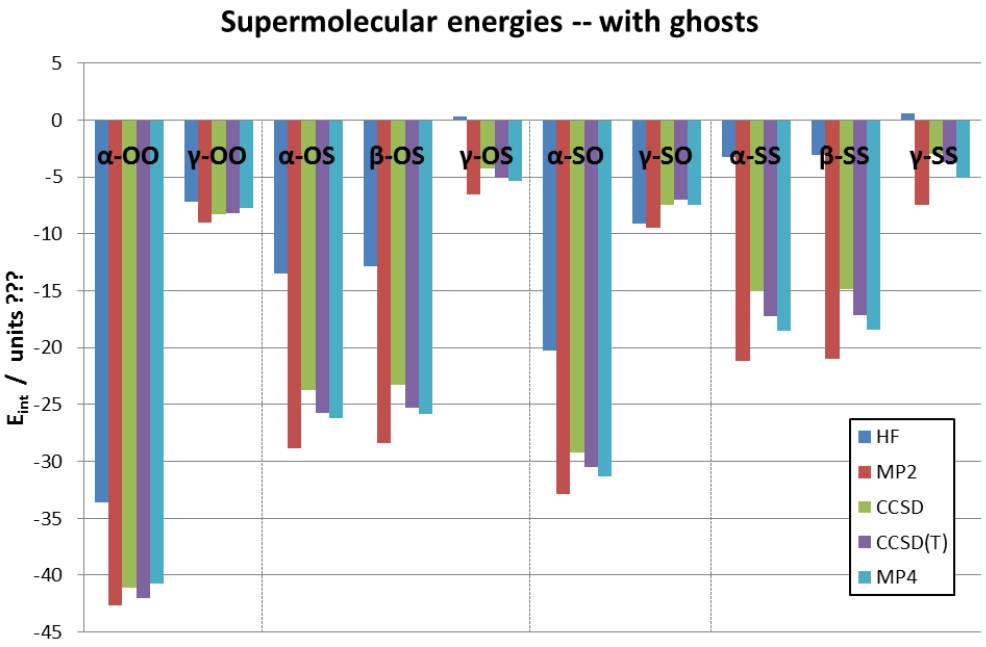

FIG. S1. Supermolecular energies with ghost atoms

TABLE S1. Supermolecular interaction energies calculated with various methods and zero-point energy correction using the aug-cc-pVDZ(-PP) basis set with midbond functions placed between the closest interacting atoms

Energy	α-OO	γ-OO	α-OS	β-OS	γ-OS	ϵ-OS	α-SO	γ-SO	α-SS	β-SS	γ-SS	ϵ-SS
$E_{\text{int}}^{\text{HF}}$	-33.61	-7.17	-13.46	-12.89	0.32	8.49	-20.22	-9.08	-3.29	-3.04	0.58	11.92
$E_{\text{int}}^{\text{MP2}}$	-42.63	-9.01	-28.84	-28.37	-6.53	-0.61	-32.83	-9.48	-21.13	-20.97	-7.45	-1.91
$E_{\text{int}}^{\text{CCSD}}$	-41.13	-8.25	-23.71	-23.26	-4.22	1.61	-29.21	-7.48	-15.06	-14.89	-2.94	2.15
$E_{\text{int}}^{\text{CCSD(T)}}$	-42.02	-8.21	-25.77	-25.31	-5.08	-0.21	-30.54	-7.02	-17.28	-17.12	-3.74	-0.51
$E_{\text{int}}^{\text{MP4}}$	-40.76	-7.75	-26.24	-25.86	-5.39	-1.14	-31.31	-7.48	-18.53	-18.39	-5.08	-1.80
$E_{\text{ZPV}}^{\text{MP2}}$	9.66	2.99	6.08	5.99	2.76	1.86	8.45	3.41	5.30	5.38	3.13	2.78

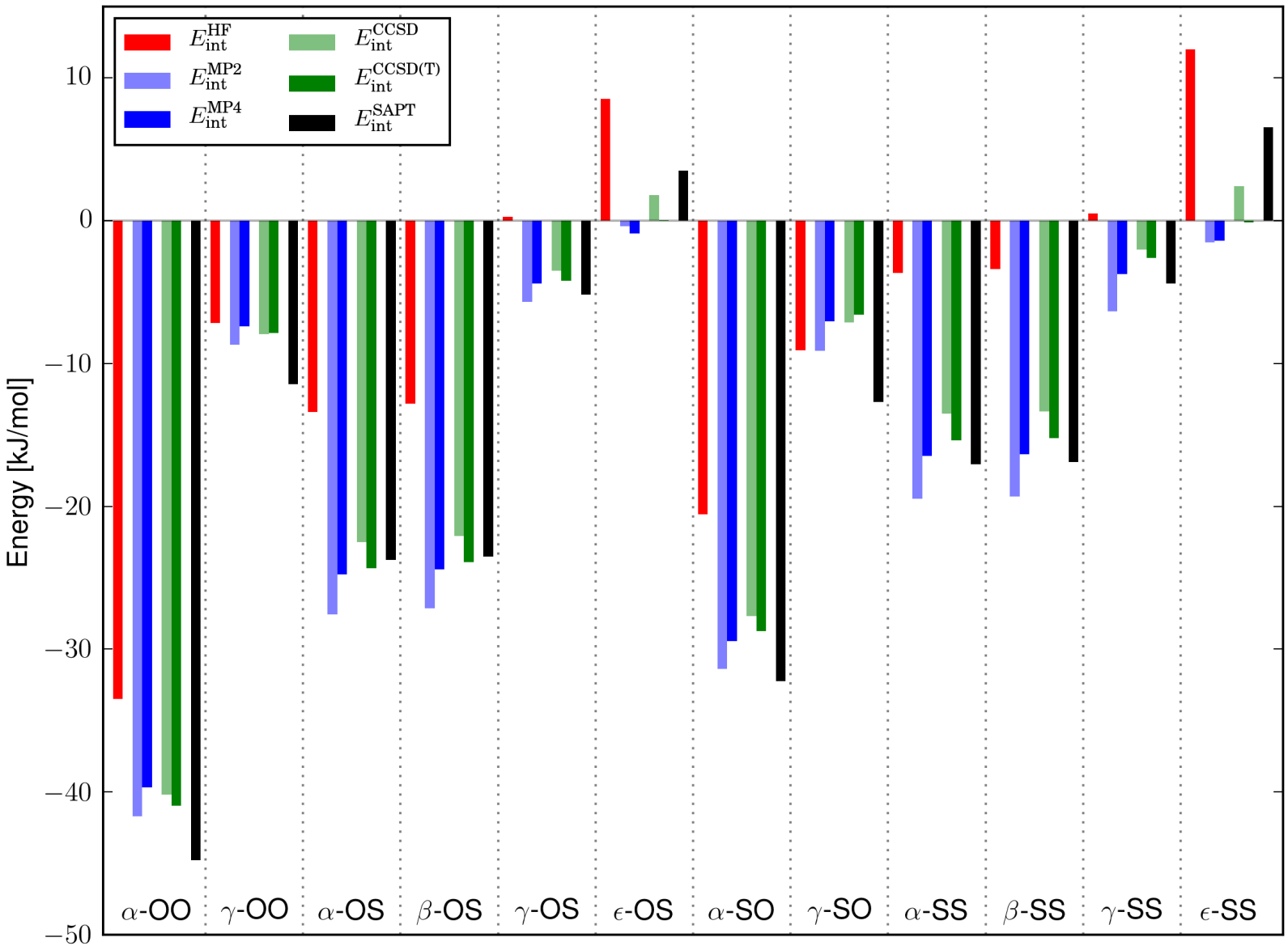

FIG. S2. Bar graph illustrating the supermolecular and SAPT interaction energies of the studied complexes

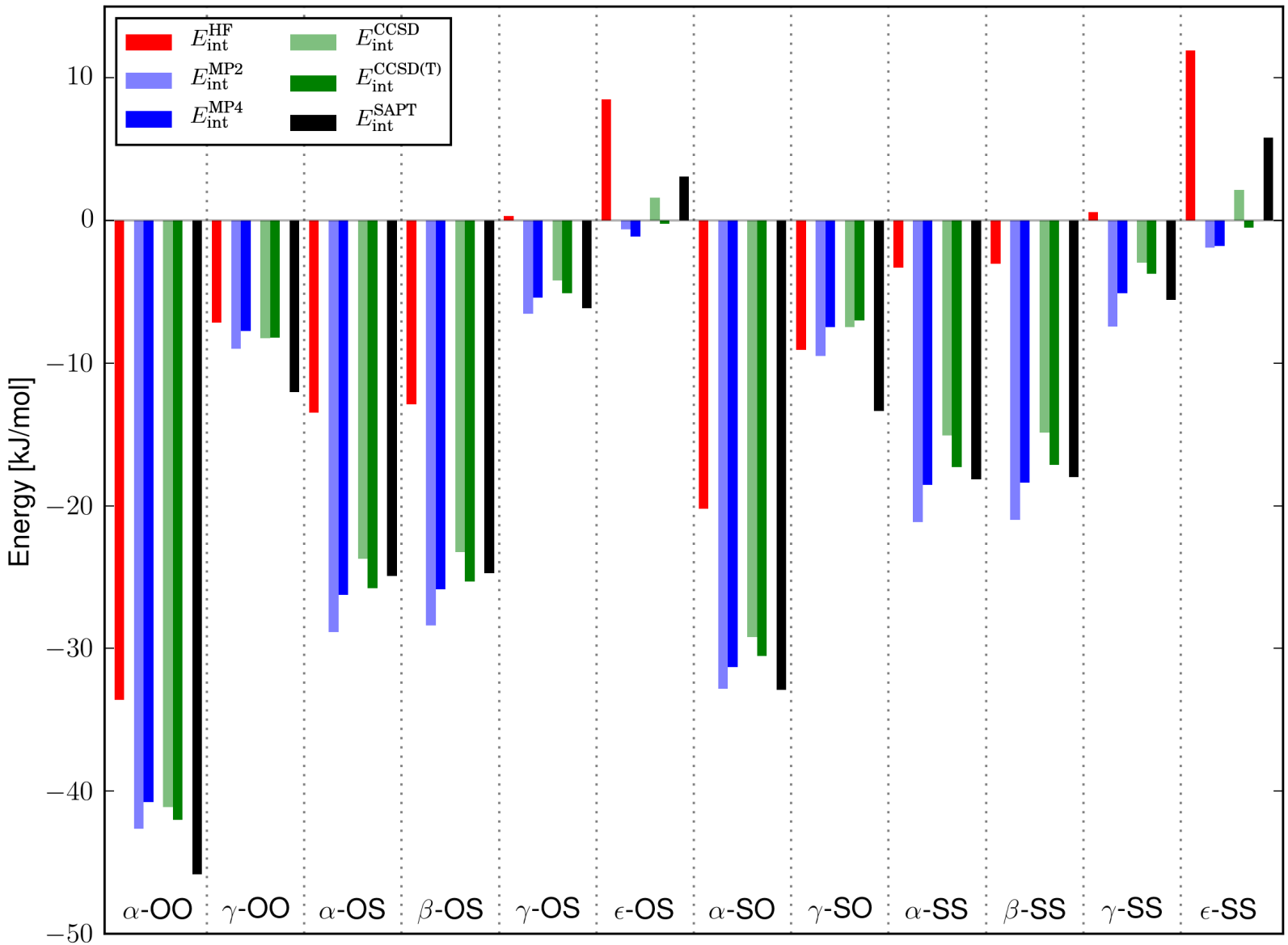

FIG. S3. Bar graph illustrating the supermolecular and SAPT interaction energies of the studied complexes with midbond functions

TABLE S2. The SAPT analysis of the intermolecular interaction energy with the midbond functions in kJ/mol

Energy	α-OO	γ-OO	α-OS	β-OS	γ-OS	ϵ-OS	α-SO	γ-SO	α-SS	β-SS	γ-SS	ϵ-SS
$E_{\text{int}}^{\text{HF}}$	-33.61	-7.17	-13.46	-12.89	0.32	8.49	-20.22	-9.08	-3.29	-3.04	0.58	11.92
E_{elst}^{1}	-82.44	-17.96	-59.05	-57.01	-11.88	2.12	-53.62	-23.49	-35.38	-35.11	-17.93	0.30
E_{exch}^{1}	77.22	17.11	73.10	70.72	18.02	10.38	50.83	24.47	46.17	46.07	29.93	20.16
E_{ind}^{2}	-42.20	-8.42	-41.12	-40.34	-9.67	-4.42	-33.03	-14.00	-33.02	-33.17	-20.05	-10.07
$E_{\text{ind-exch}}^{2}$	23.86	5.07	25.27	24.72	7.14	2.47	21.94	9.29	24.32	24.46	15.87	6.57
E_{disp}^{2}	-28.31	-9.67	-29.62	-29.16	-11.82	-8.44	-23.70	-12.28	-25.03	-25.07	-16.70	-12.89
$E_{\text{disp-exch}}^{2}$	6.05	1.84	6.51	6.36	2.07	0.96	4.68	2.65	4.82	4.83	3.32	1.75
E_{tot}^{1}	-5.22	-0.84	14.04	13.71	6.14	12.50	-2.79	0.98	10.79	10.96	12.01	20.46
E_{tot}^{2}	-40.60	-11.17	-38.97	-38.42	-12.28	-9.43	-30.10	-14.34	-28.92	-28.95	-17.56	-14.64
$\delta E_{\text{int,resp}}^{\text{HF}}$	-10.05	-2.99	-11.65	-10.99	-3.30	-2.06	-6.35	-5.36	-5.38	-5.29	-7.25	-5.05
$E_{\text{int}}^{\text{SAPT}}$	-45.82	-12.01	-24.92	-24.71	-6.14	3.07	-32.89	-13.35	-18.13	-17.99	-5.55	5.82
$E_{\text{elst}}/E_{\text{int}}^{\text{SAPT}}$	1.80	1.50	2.37	2.31	1.93	0.69	1.63	1.76	1.95	1.95	3.23	0.05
$E_{\text{exch}}/E_{\text{int}}^{\text{SAPT}}$	-1.69	-1.42	-2.93	-2.86	-2.93	3.38	-1.55	-1.83	-2.55	-2.56	-5.39	3.46
$E_{\text{ind}}/E_{\text{int}}^{\text{SAPT}}$	0.40	0.28	0.64	0.63	0.41	-0.64	0.34	0.35	0.48	0.48	0.75	-0.60
$E_{\text{disp}}/E_{\text{int}}^{\text{SAPT}}$	0.49	0.65	0.93	0.92	1.59	-2.44	0.58	0.72	1.11	1.13	2.41	-1.91

TABLE S3. The anharmonic wavenumbers (cm^{-1}) and integrated intensities ($km \cdot mol^{-1}$) of infrared spectra of the complexes of HXeOH calculated using MP2/aug-cc-pVDZ(-PP) method. Zeros in this table mean negative anharmonic values which were positive within harmonic approximation

HXeOH		α-OO			γ-OO			α-OS			β-OS			γ-OS			ϵ-OS		
$\bar{\nu}$	I	$\bar{\nu}$	$\Delta\nu$*	I	$\bar{\nu}$	$\Delta\nu$*	I	$\bar{\nu}$	$\Delta\nu$*	I	$\bar{\nu}$	$\Delta\nu$*	I	$\bar{\nu}$	$\Delta\nu$*	I	$\bar{\nu}$	$\Delta\nu$*	I
3609	55	3708		55	3729		89	3591		60	3595		62	3600		56	3589		80
		3600		55	3609		4	2666		1	2665		2	2673		0	2667		6
		3239		679	3606		50	2276		440	2292		349	2651		2	2630		4
1721	1087	1812	91	826	1783	62	402	1782	61	894	1781	60	891	1728	7	532	1686	-35	1186
		1605		57	1574		67	1172		3	1172		5	1164		0	1163		1
817	6	754		41	768		3	773		1	768		1	766		4	787		8
		732		33	640		0	581		26	593		13	628		4	633		12
630	0	599		1	579		6	563		73	546		9	584		2	570		2
597	3	554		5	425		168	518		62	494		101	427		177	438		127
437	130	443		91	112		58	413		129	417		103	96		0	0		0
		408		132	87		246	188		17	197		19	91		22	136		1
		218		59	58		28	137		54	139		32	43		13	28		7
		210		260	0		0	118		162	33		56	0		0	0		0
		99		80	25		374	97		22	102		92	14		4	0		0
		65		24	0		0	40		5	35		5	0		0	0		0

* The difference between the wavenumber in the complex and the HXeOH monomer

TABLE S4. The anharmonic wavenumbers (cm^{-1}) and integrated intensities ($km \cdot mol^{-1}$) of infrared spectra of the complexes of HXeSH calculated using MP2/aug-cc-pVDZ(-PP) method. Zeros in this table mean negative anharmonic values which were positive within harmonic approximation

HXeSH		α-SO			γ-SO			α-SS			β-SS			γ-SS			ϵ-SS		
$\bar{\nu}$	I	$\bar{\nu}$	$\Delta\nu$*	I	$\bar{\nu}$	$\Delta\nu$*	I	$\bar{\nu}$	$\Delta\nu$*	I	$\bar{\nu}$	$\Delta\nu$*	I	$\bar{\nu}$	$\Delta\nu$*	I	$\bar{\nu}$	$\Delta\nu$*	I
		3691		75	3724		70	2664		1	2664		1	2671		1	2665		5
		3387		367	3603		10	2626		5	2626		5	2649		6	2630		6
2634	7	2628		5	2631		7	2482		267	2482		267	2631		4	2577		38
1375	2520	1584	209	1868	1499	124	652	1436	61	2317	1436	61	2322	1385	10	1209	1365	-10	2583
		1488	113	3043	1565	190	809	1167		4	1169		4	1164		0	1146		3
626	3	601		12	626		3	601		3	605		2	615		4	511		5
523	0	536		47	547		1	509		0	508		0	544		0	432		0
		512		2	444		0	443		1	443		1	454		1	372		2
460	2	442		2	240		77	363		25	360		20	239		87	246		42
		349		132	131		79	243		53	221		534	117		0	4		1
248	33	242		49	0		0	211		20	240		255	118		21	112		14
		125		25	0		0	113		19	118		4	40		12	39		2
		136		219	0		0	95		17	95		5	1		10	0		0
		140		6	0		0	76		11	70		25	0		0	0		0
		74		11	0		0	46		4	44		5	0		0	0		0

* The difference between the wavenumber in the complex and the HXeSH monomer

TABLE S5. The coordinates of atoms in α-OO given in Å.

Xe	0.636300	-0.089621	0.000183
H	1.883260	-1.228470	-0.000017
O	-1.059593	1.398812	-0.104664
H	-1.044224	1.991225	0.665954
H	-2.254909	0.106888	-0.010134
O	-2.616797	-0.810405	0.051414
H	-3.533205	-0.737369	-0.239697

TABLE S6. The coordinates of atoms in γ-OO given in Å.

O	-2.538418	0.000141	-0.116017
H	-2.936657	-0.000691	0.770751
Xe	-0.302212	-0.000012	0.002766
H	1.394149	-0.000028	-0.008039
O	3.699833	-0.000029	0.022428
H	4.285068	0.762103	-0.081213
H	4.285564	-0.761654	-0.082136

TABLE S7. The coordinates of atoms in α-OS given in Å.

Xe	-1.018107	-0.145442	0.000949
H	-2.072126	-1.472491	0.008652
O	0.433097	1.567320	0.088400
H	0.233036	2.236024	-0.589282
H	2.026101	0.604912	-0.038415
S	2.999957	-0.365834	-0.084590
H	3.326697	-0.199772	1.214049

TABLE S8. The coordinates of atoms in β-OS given in Å.

Xe	1.015940	-0.147052	0.002219
H	2.062147	-1.480621	0.001074
O	-0.428253	1.570484	-0.089160
H	-0.190846	2.268654	0.545045
H	-2.039408	0.621983	0.000664
S	-3.007115	-0.351116	-0.076093
O	-3.152791	-0.415219	1.264159

TABLE S9. The coordinates of atoms in γ-OS given in Å.

O	2.993155	0.149314	0.000016
H	3.397627	-0.735084	-0.000036
Xe	0.767336	-0.010181	-0.000004
H	-0.939900	-0.031027	-0.000013
S	-3.753429	-0.095841	-0.000008
H	-3.892172	0.827554	-0.975282
H	-3.892058	0.827285	0.975536

TABLE S10. The coordinates of atoms in ε-OS given in Å.

O	3.080119	0.059722	-0.008596
H	3.414390	-0.746660	0.422247
Xe	0.873760	0.008005	-0.008881
H	-0.848166	0.052256	-0.052970
S	-4.197846	-0.092081	-0.002659
H	-2.853025	0.038144	-0.043835
H	-4.371685	1.219537	0.265453

TABLE S11. The coordinates of atoms in α-SO given in Å.

S	1.651068	-1.244755	-0.081201
Xe	-0.829579	0.014997	-0.000876
H	1.668520	-1.381502	1.266277
H	-2.370283	0.805000	0.029880
H	2.053858	1.070834	-0.020607
O	1.798724	2.015201	0.012057
H	2.638295	2.490288	-0.025502

TABLE S12. The coordinates of atoms in γ-SO given in Å.

S	2.729592	-0.056266	-0.000009
Xe	-0.061712	-0.012926	-0.000012
H	2.791161	1.296518	0.000517
H	-1.791027	-0.007131	-0.000020
O	-4.015967	0.043519	0.000034
H	-4.606716	-0.019173	-0.762655
H	-4.606686	-0.020089	0.762671

TABLE S13. The coordinates of atoms in α-SS given in Å.

S	-0.287110	2.045480	-0.079692
Xe	1.026325	-0.391776	-0.002807
H	-0.233920	2.161560	1.269118
H	1.844529	-1.931428	0.024469
H	-2.199033	0.423246	0.015624
S	-2.935522	-0.722910	0.083724
H	-3.271004	-0.658614	-1.222171

TABLE S14. The coordinates of atoms in β-SS given in Å.

S	0.285818	2.046932	-0.082741
Xe	-1.026104	-0.391285	0.001894
H	0.279119	2.134131	1.269290
H	-1.844262	-1.930833	0.035100
S	2.934857	-0.727980	-0.076987
H	2.201186	0.422019	-0.081986
H	3.242769	-0.599188	1.230971

TABLE S15. The coordinates of atoms in γ-SS given in Å.

S	-3.162198	-0.057026	0.000002
Xe	-0.378908	-0.012645	0.000000
H	-3.216956	1.296141	-0.000020
H	1.373389	-0.005067	-0.000001
S	4.036530	0.119763	-0.000007
H	4.157654	-0.805945	0.975917
H	4.157653	-0.806082	-0.975801

TABLE S16. The coordinates of atoms in ε-SS given in Å.

S	-3.220161	-0.042208	-0.024788
H	-3.258081	1.050934	0.774408
Xe	-0.483378	-0.011311	-0.010379
H	1.305075	-0.007764	-0.011681
S	4.490836	0.073765	-0.037658
H	3.135660	0.023968	-0.026981
H	4.588955	-0.961256	0.823856

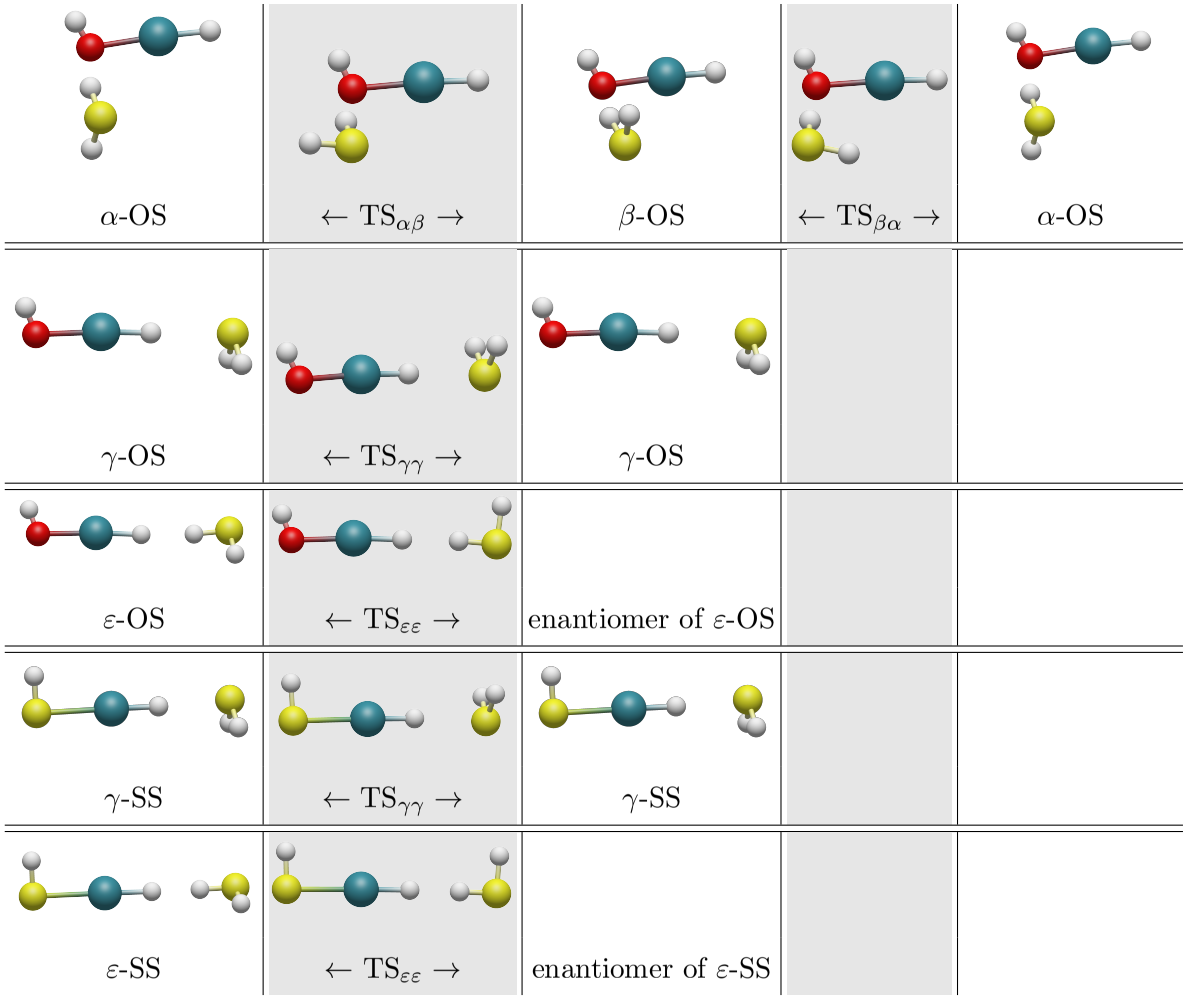

FIG. S4. Transition states between various complex conformers

TABLE S17. The coordinates of atoms in $TS_{\alpha\beta}$ given in Å.

Xe	1.018350	-0.142748	0.004705
H	2.067191	-1.477580	0.017267
O	-0.410312	1.582909	-0.122473
H	-0.324210	2.147145	0.665904
H	-2.009083	0.570033	-0.060329
S	-2.967996	-0.415258	-0.012359
H	-3.954356	0.449675	0.300605

TABLE S18. The coordinates of atoms in $TS_{\beta\alpha}$ given in Å.

Xe	1.080469	-0.129648	0.003679
H	2.235445	-1.376812	0.013852
O	-0.476880	1.473358	-0.119929
H	-0.440973	2.035084	0.674362
H	-2.100954	0.497911	-0.067319
S	-3.230209	-0.281892	0.017383
H	-2.540435	-1.431812	-0.138253

TABLE S19. The coordinates of atoms in $TS_{\gamma\gamma}$(OS) given in Å.

O	-2.998250	-0.104586	-0.005283
H	-3.380911	0.787285	0.057168
Xe	-0.769355	0.001480	-0.000329
H	0.937850	-0.016985	-0.003380
S	3.757031	-0.101887	-0.012246
H	3.932150	0.928609	-0.866896
H	3.929595	0.688066	1.069062

TABLE S20. The coordinates of atoms in $TS_{\varepsilon\varepsilon}$(OS) given in Å.

O	3.078491	-0.116502	0.000006
H	3.443294	0.786007	0.000002
Xe	0.874755	0.003425	-0.000001
H	-0.848373	0.002664	-0.000006
S	-4.203910	-0.081562	0.000001
H	-2.854768	0.002058	-0.000006
H	-4.342298	1.261319	0.000005

TABLE S21. The coordinates of atoms in $TS_{\gamma\gamma}$(SS) given in Å.

S	-3.162431	-0.066879	0.000001
H	-3.223527	1.286064	-0.000078
Xe	-0.379456	-0.006120	0.000002
H	1.372712	0.009548	0.000004
S	4.038874	-0.097047	0.000027
H	4.159138	0.828560	-0.976093
H	4.159199	0.829112	0.975616

TABLE S22. The coordinates of atoms in $TS_{\varepsilon\varepsilon}$(SS) given in Å.

S	-3.220485	-0.055996	-0.000048
H	-3.264009	1.297979	0.000212
Xe	-0.483727	-0.011163	-0.000009
H	1.304697	-0.001061	0.000014
S	4.492873	-0.065792	0.000047
H	3.137320	-0.026797	0.000034
H	4.585043	1.281274	0.000234