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

Supporting Information for:

Computational insight into hydrogen persulfide and a new additive model for chemical and biological simulations

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Table S1. Molecular properties of H_2S_2 and H_2S.

Molecule (conformer)	Property	MP2(full)/ 6-311++G(d,p)	CCSD(T)/ 6-311++G(3df,3pd)	CCSD(T)/aug-cc-pVXZ		
				X=D	X=T	X=Q
H_2S_2 (**pa**)	r_{SH} (Å)	1.336	1.342	1.359	1.346	1.343
	r_{SS} (Å)	2.082	2.070	2.121	2.084	2.067
	$r_{S...H}$ (Å)	2.627	2.620	2.658	2.627	2.619
	$r_{H...H}$ (Å)	3.097	3.091	3.123	3.093	3.092
	θ_{HSS} (deg)	98.0	98.1	97.1	97.7	98.1
	φ_{HSSH} (deg)	91.0	90.5	91.1	90.7	90.7
	Dipole (D)	1.53	1.22	1.29	1.25	1.24
	α (Å^3)	5.26	6.33	6.53	6.58	6.56
	IPV (eV)	9.93	10.01	9.90	10.07	10.13
	S–S BDE (kcal/mol)	51.2	58.0	51.2	58.3	61.2
	S–H BDE(kcal/mol)	69.4	71.7	69.4	71.9	72.4
	Vibrational frequencies (cm^{-1})					
	ν_1 (sym. SH str.)	2783	2683	2656	2668	2671
	ν_2 (sym. HSS-bend.)	923	902	879	894	901
	ν_3 (SS-stretch)	516	516	488	512	523
	ν_4 (SS-torsion)	412	435	417	424	433
	ν_5 (antisym. SH-str.)	2785	2686	2658	2670	2676
	ν_6 (antisym. HSS-bend.)	916	901	873	892	899
H_2S_2 (**pb**)	r_{SH} (Å)	1.333	1.337	1.356	1.342	1.339
	r_{SS} (Å)	2.136	2.128	2.176	2.139	2.123
	$r_{S...H}$ (Å)	2.641	2.633	2.680	2.640	2.628
	$r_{H...H}$ (Å)	2.433	2.418	2.456	2.415	2.409
	θ_{HSS} (deg)	96.4	96.2	95.9	95.9	96.1
	Φ_{HSSH} (deg)	0.0	0.0	0.0	0.0	0.0
	Dipole (D)	2.14	1.67	1.77	1.71	1.70
	α (Å^3)	5.29	6.39	6.59	6.65	6.64
	IPV (eV)	8.61	8.85	8.78	8.92	8.96
	ΔE (kcal/mol)[a]	7.2	7.2	6.8	6.9	7.1
	S–S BDE (kcal/mol)	44.0	50.8	44.4	51.4	54.1
	S–H BDE (kcal/mol)	62.2	64.5	62.6	65.0	65.3
H_2S_2 (**pc**)	r_{SH} (Å)	1.333	1.338	1.356	1.343	1.340
	r_{SS} (Å)	2.126	2.116	2.164	2.127	2.112
	$r_{S...H}$ (Å)	2.563	2.559	2.606	2.568	2.556
	$r_{H...H}$ (Å)	3.490	3.494	3.547	3.504	3.493
	θ_{HSS} (deg)	92.8	92.8	92.6	92.7	92.8
	Φ_{HSSH} (deg)	180.0	180.0	180.0	180.0	180.0
	Dipole (D)	0.0	0.0	0.0	0.0	0.0
	α (Å^3)	5.35	6.40	6.61	6.67	6.65
	IPV (eV)	8.56	8.81	8.74	8.88	8.92
	ΔE (kcal/mol)[a]	4.7	5.1	4.8	4.8	5.0
	S–S BDE (kcal/mol)	46.6	52.9	46.4	53.4	56.1
	S–H BDE (kcal/mol)	64.7	66.6	64.6	67.1	67.3
H_2S	r_{SH} (Å)	1.333	1.338	1.356	1.342	1.340
	θ_{HSS} (deg)	92.1	92.5	92.4	92.3	92.3
	Dipole (D)	1.37	1.06	1.14	1.09	1.08
	α (Å^3)	2.65	3.41	3.50	3.60	3.62
	IPV (eV)	9.99	10.32	10.18	10.39	10.45
	S–H BDE (kcal/mol)	83.3	88.6	84.4	88.3	89.5

[a] Relative energy ($\Delta E = E_{\mathbf{pb/pc}} - E_{\mathbf{pa}}$) corrected for ZPE

Note: Properties calculated with MP2(full)/6-311++G(d,p) and CCSD(T)/aug-cc-pVDZ show the least agreement with the experimental properties reported in Table 1 of the main text.

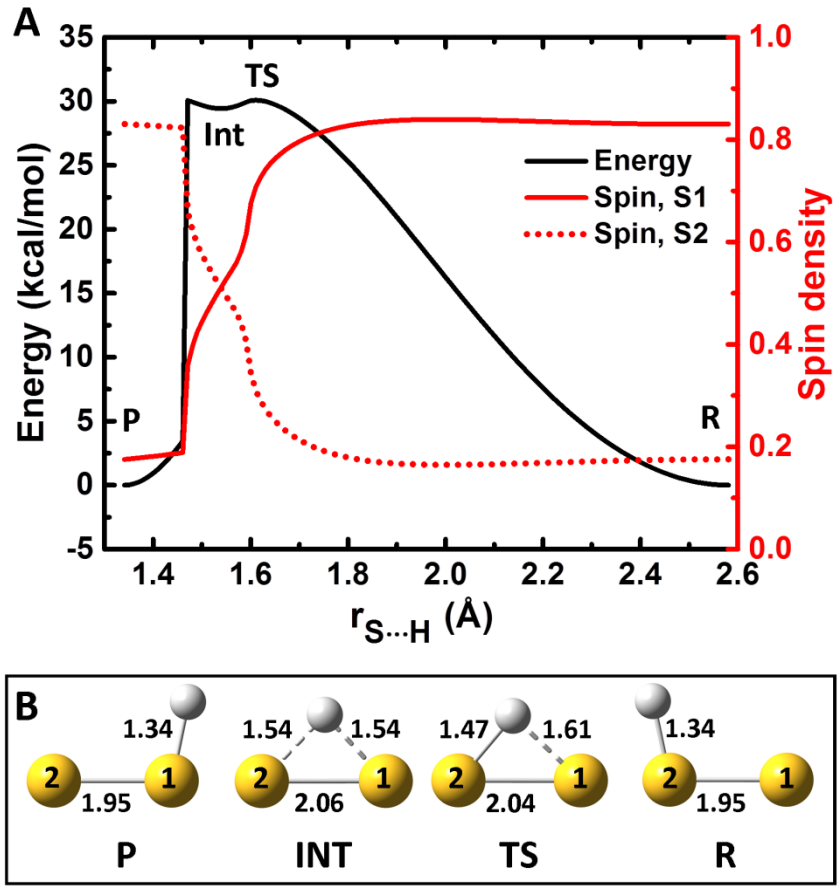

Figure S1. Resonance in the perthiyl radical (HSS˙ ↔ ˙SSH). (A) Relaxed scan of the distance between S1 and H from 2.58 to 1.34 Å, in 0.01 Å increments. The black curve (scale on the left) show the change in energy and red curves (scale on the right) show the radical density on each S atom along the scan. (B) Geomety and structural properties of the reactant (R), product (P), transition state (TS), and intermediate (Int) observed during the scan.

Table S2. Binding energies (E and E^{CP}, kcal/mol) for the $(H_2S_2)_2$ and $(H_2S_2)_3$ complexes displayed in Figure 2 of the main text.[a]

Complex	Conformer	MP2(full)/ 6-311++G(d,p)		CCSD(T)/ 6-311++G(3df,3pd)		CCSD(T)/ aug-cc-pV5Z[b]	
		E	E^{CP}	E	E^{CP}	E	E^{CP}
$(H_2S_2)_2$	**2pa**	-3.6	0.0	-3.4	-1.7	-2.9	-2.8
	2pb	-3.9	-1.1	-4.2	-2.6	-3.5	-3.3
	2pc	-4.0	-0.3	-4.2	-2.4	-3.8	-3.6
	2pd	-5.0	-1.2	-4.5	-2.7	-3.9	-3.7
	2pe	-4.4	-0.5	-4.7	-2.9	-4.4	-4.2
	2pf	-4.4	-0.3	-5.2	-3.2	-4.9	-4.7
$(H_2S_2)_3$	**3pa**	-8.2	-0.5	-7.3	-3.5		
	3pb	-9.0	-1.3	-8.1	-4.2		
	3pc	-10.2	-1.6	-9.3	-5.0		
	3pd	-8.7	-0.9	-9.2	-5.4		
	3pe	-9.6	-1.4	-9.8	-5.4		
	3pf	-9.6	-1.0	-9.8	-5.5		
	3pg	-9.6	-1.4	-9.9	-5.6		
	3ph	-9.6	-0.8	-10.0	-5.6		
	3pi	-9.2	-1.2	-9.8	-5.8		
	3pj	-10.2	-1.3	-10.2	-5.8		
	3pk	-9.7	-1.3	-10.3	-5.9		
	3pl	-9.6	-1.5	-10.6	-6.2		
	3pm	-10.0	-1.5	-10.2	-5.9		
	3pn	-10.9	-1.8	-10.8	-6.3		
	3po	-10.3	-1.5	-10.7	-6.3		
	3pp	-10.0	-1.7	-11.1	-6.7		

[a] Energies are calculated for MP2(full)/6-311++G(3df,3pd) geometries. [b] Could not be performed on the trimer as the calculations are computationally prohibitive.

Note: MP2(full)/6-311++G(d,p) predict very low BSSE-corrected binding energies due to very large BSSE (72–99 % of the E values). This highlights the criticalness of have large diffuse functions for studying these highly polarizable clusters. Binding energies calculated with CCSD(T)/6-311++G(3df,3pd) are in good agreement with those from MP2(full)/6-311++G(3df,3pd) and from the optimized additive model for H_2S_2 (Table 1 of the main text).

Table S3. Binding energies (E and E^{CP}, kcal/mol) for the $H_2S_2 \cdot H_2O$, $(H_2O)_2 \cdot H_2S_2$, and $(H_2S_2)_2 \cdot H_2O$ complexes shown in Figure 3 of the main text.[a]

Complex	Structure	MP2(full)/ 6-311++G(d,p)		CCSD(T)/ 6-311++G(3df,3pd)		CCSD(T)/ aug-cc-pV5Z	
		E	E^{CP}	E	E^{CP}	E	E^{CP}
$H_2S_2 \cdot H_2O$	**pwa**	-3.3	-1.9	-2.9	-2.2	-2.6	-2.5
	pwb	-4.8	-2.8	-4.6	-3.6	-4.4	-4.2
$(H_2O)_2 \cdot H_2S_2$	**2wpa**	-8.0	-4.5	-7.6	-5.6		
	2wpb	-9.6	-5.1	-9.2	-6.9		
	2wpc	-9.9	-5.4	-9.4	-7.2		
	2wpd	-9.8	-5.8	-9.4	-7.3		
	2wpe	-11.0	-6.1	-10.2	-7.9		
	2wpf	-11.8	-7.7	-10.3	-8.3		
	2wpg	-12.8	-8.1	-11.7	-9.4		
	2wph	-13.0	-8.2	-11.8	-9.5		
	2wpi	-13.2	-8.3	-12.0	-9.7		
	2wpj	-13.6	-8.3	-12.3	-10.0		
	2wpk	-14.7	-9.3	-13.1	-10.6		
	2wpl	-15.1	-9.6	-13.5	-10.9		
$(H_2S_2)_2 \cdot H_2O$	**2pwa**	-7.9	-2.8	-7.5	-4.7		
	2pwb	-8.3	-2.0	-8.0	-4.9		
	2pwc	-7.2	-1.8	-7.7	-4.9		
	2pwd	-8.2	-4.2	-8.0	-5.8		
	2pwe	-8.5	-2.3	-8.4	-5.2		
	2pwf	-8.7	-0.9	-8.1	-4.6		
	2pwg	-8.8	-2.9	-8.1	-5.3		
	2pwh	-8.5	-2.8	-8.2	-5.3		
	2pwi	-8.6	-2.6	-8.9	-5.6		
	2pwj	-10.2	-3.8	-8.6	-5.7		
	2pwk	-9.3	-2.8	-8.9	-5.7		
	2pwl	-10.2	-3.4	-9.0	-6.0		
	2pwm	-8.8	-3.0	-8.9	-5.9		
	2pwn	-9.8	-3.5	-9.4	-6.3		
	2pwo	-9.6	-2.4	-9.2	-5.9		
	2pwp	-10.1	-3.3	-9.3	-6.1		
	2pwq	-10.6	-4.7	-9.4	-6.6		
	2pwr	-10.3	-4.1	-10.0	-6.8		
	2pws	-9.6	-3.5	-9.6	-6.6		
	2pwt	-10.5	-4.4	-10.1	-6.9		
	2pwu	-12.4	-5.6	-11.0	-8.0		
	2pwv	-12.4	-5.4	-11.4	-8.2		

[a] Energies are calculated for MP2(full)/6-311++G(3df,3pd) geometries. [b] Could not be performed on the trimers as the calculations are computationally prohibitive.

Table S4. Binding energies (E and E^{CP}, kcal/mol) for H_2S_2 complexes presented in Figure 4.[a]

Ligand	Conformer	MP2(full)/ 6-311++G(d,p)		CCSD(T)/ 6-311++G(3df,3pd)	
		E	E^{CP}	E	E^{CP}
Ethane	**1a**	-1.4	0.1	-1.8	-0.7
	1b	-2.5	0.1	-2.4	-1.0
Acetamide	**2a**	-4.5	-0.9	-4.3	-2.5
	2b	-7.4	-3.8	-6.8	-5.1
	2c	-8.5	-5.0	-8.5	-6.7
NMA	**3a**	-6.0	-1.1	-5.1	-2.7
	3b	-6.8	-1.9	-5.6	-3.4
	3c	-7.8	-4.1	-7.1	-5.3
	3d	-8.2	-3.3	-7.4	-5.1
Methylamine	**4a**	-3.1	-0.3	-3.1	-1.7
	4b	-7.5	-4.2	-6.3	-4.8
Methylammonium$^+$	**5a**	-12.0	-8.5	-12.1	-10.4
	5b	-14.2	-10.7	-13.9	-12.1
	5c	-14.3	-10.8	-13.9	-12.2
Methylguanidinum	**6a**	-10.9	-6.4	-10.3	-8.0
	6b	-11.4	-7.2	-11.4	-9.2
	6c	-12.1	-7.5	-11.7	-9.4
	6d	-13.7	-9.3	-12.9	-10.8
Methane thiol	**7a**	-3.2	0.1	-3.1	-1.6
	7b	-4.9	-1.6	-4.6	-3.0
	7c	-4.8	-1.3	-4.9	-3.2
Methanethiolate	**8a**	-15.8	-10.4	-14.6	-12.2
	8b	-17.3	-11.1	-15.9	-13.2
	8c	-19.2	-13.5	-17.5	-15.1
	8d	-31.7	-24.1	-29.1	-26.0
DMS	**9a**	-3.5	-0.0	-3.0	-1.3
	9b	-4.8	-1.5	-4.5	-2.9
	9c	-5.6	-1.8	-5.6	-3.5
DMDS	**10a**	-5.1	-0.8	-4.8	-2.7
	10b	-5.3	-1.2	-5.1	-2.9
	10c	-5.9	-1.1	-5.6	-3.1
	10d	-5.7	-1.3	-5.4	-3.2
Methanol	**11a**	-3.6	-1.1	-3.8	-2.4
	11b	-5.7	-2.9	-4.6	-3.3
	11c	-5.6	-3.1	-5.1	-3.8
	11d	-5.7	-2.6	-5.6	-4.1
Acetic acid	**12a**	-5.3	-1.4	-4.4	-2.6
	12b	-5.7	-2.6	-5.3	-3.8
	12c	-8.4	-4.9	-8.4	-6.6
Acetate	**13a**	-18.8	-14.4	-17.5	-15.6
	13b	-25.4	-20.0	-23.5	-21.1
	13c	-31.4	-25.7	-30.0	-27.3
	13d	-34.3	-27.4	-32.0	-29.0

[a] Energies are calculated for MP2(full)/6-311++G(3df,3pd) geometries

Table S5. Binding energies (E and E^{CP}, kcal/mol) for the H_2S_2 complexes presented in Figure 5.[a]

Ligand	Conformer	MP2(full)/ 6-311++G(d,p)		CCSD(T)/ 6-311++G(3df,3pd)	
		E	E^{CP}	E	E^{CP}
Toluene	**14a**	-8.81	-2.9	-6.4	-3.5
3-Methylindole	**15a**	-10.4	-3.6	-6.9	-3.8
	15b	-11.7	-4.3	-7.7	-4.5
	15c	-11.7	-3.9	-7.7	-4.2
	15d	-13.0	-4.7	-8.6	-5.0
	15e	-13.2	-5.0	-8.7	-5.1
4-Methylphenol	**16a**	-7.8	-1.2	-4.7	-1.9
	16b	-7.6	-1.1	-4.9	-1.9
	16c	-9.3	-2.9	-6.5	-3.6
	16d	-10.0	-3.3	-7.0	-4.0
	16e	-10.1	-3.3	-7.1	-4.0
4-Methylimidazole	**17a**	-6.9	-1.1	-4.6	-2.1
	17b	-7.8	-2.6	-5.8	-3.4
	17c	-8.1	-3.2	-6.0	-3.9
	17d	-8.3	-3.2	-6.2	-3.8
	17e	-8.4	-5.0	-7.1	-5.5
	17f	-9.9	-3.9	-7.2	-4.7
4-Methylimidazolium	**18a**	-10.9	-6.5	-9.9	-8.0
	18b	-12.7	-8.6	-11.4	-9.3
	18c	-12.6	-8.3	-11.4	-9.3
	18d	-12.9	-8.8	-11.5	-9.7
4-Methylphenolate	**19a**	-23.3	-15.0	-19.9	-16.3
	19b	-29.3	-21.2	-25.9	-22.7
	19c	-29.1	-22.5	-26.3	-23.6

[a] Energies are calculated for MP2(full)/6-311++G(3df,3pd) geometries

Note: Freezing the core electrons has very little effect on MP2 calculations. With the same basis set, it results in a slightly weaker interaction (most likely because of lower dispersion interactions) and a slightly lower BSSE (anticipated for fewer electronic degrees of freedom), and these slight differences compensate each other. For example geometry optimization and interaction energy calculations for conformers **2pa** and **2pf** of $(H_2S_2)_2$, conformer **2c** of H_2S_2-acetamide, and conformer **5c** of H_2S_2-methylammonium with MP2(fc)/6-311++G(3df,3pd) result in structures with ≤ 0.02 Å longer H-bonds and ≤ 0.4 kcal/mol smaller BSSE, and the same BSSE-corrected interaction energies as those determined with MP2(full)/ 6-311++G(3df,3pd).

Table S6. Density of liquid H_2S_2 calculated with the optimized additive model vs *T* and *p*

T (K)	*p* (atm)	density (g/cm^3)
233.15	0.0018	1.382
243.15	0.0043	1.370
253.15	0.0094	1.359
263.15	0.0192	1.348
273.15	0.0381	1.337
283.15	0.0707	1.326
293.15	0.1256	1.315
303.15	0.2103	1.303
313.15	0.3459	1.291
323.15	0.5547	1.281
333.15	0.8523	1.269

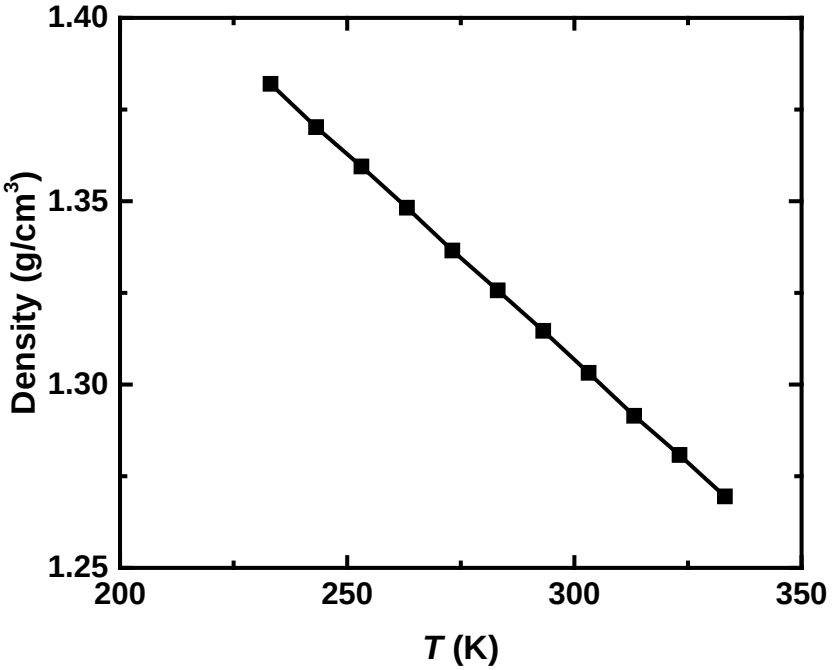

Figure S2. Calculated density of liquid H_2S_2 vs temperature. Data from Table S6.

Atomic coordinates of the structures presented in Figure 1–5 of the main text

Optimized conformers for the H_2S_2 monomer (Fig. 1A)

Conformer Pa

S	0.000000000	1.024270000	-0.054576000
H	0.939714000	1.214031000	0.873214000
S	0.000000000	-1.024270000	-0.054576000
H	-0.939714000	-1.214031000	0.873214000

Conformer Pb

S	0.000000000	1.052304000	-0.077754000
H	0.000000000	1.200294000	1.244069000
S	0.000000000	-1.052304000	-0.077754000
H	0.000000000	-1.200294000	1.244069000

Conformer Pc

S	0.000000000	1.046740000	0.000000000
H	1.329936000	1.110040000	0.000001000
S	0.000000000	-1.046740000	0.000000000
H	-1.329936000	-1.110040000	0.000001000

Optimized conformers for the $(H_2S_2)_2$ dimer (Fig. 2A)

Conformer 2pa

S	-1.600006000	0.772241000	0.695091000
H	-2.587910000	0.399057000	1.512437000
S	-1.760617000	-0.758918000	-0.659354000
H	-2.609654000	-0.165837000	-1.500983000
S	1.671044000	0.683689000	-0.765664000
H	2.386282000	1.622384000	-0.142078000
S	1.821176000	-0.783335000	0.655207000
H	0.705742000	-0.474439000	1.326143000

Conformer 2pb

S	-2.025879000	1.025425000	0.000607000
H	-0.713305000	1.256026000	0.113661000
S	-1.928205000	-1.022764000	-0.083250000
H	-2.015715000	-1.277590000	1.224226000
S	1.928678000	1.022507000	0.086135000
H	2.013159000	1.280971000	-1.220837000
S	2.025597000	-1.025356000	-0.003664000
H	0.712805000	-1.256411000	-0.114291000

Conformer 2pc

S	-1.803964000	-0.821259000	-0.626142000
H	-0.658876000	-0.550111000	-1.263580000
S	-1.705402000	0.705214000	0.737608000
H	-2.414276000	1.610852000	0.059280000
S	1.782326000	-0.735708000	0.671139000
H	2.581839000	-0.097771000	1.528427000
S	1.717975000	0.707174000	-0.782738000
H	0.636356000	1.350291000	-0.321998000

Conformer 2pd

S	1.917466000	-0.916847000	-0.489036000
H	0.627161000	-1.221315000	-0.309365000
S	1.872670000	0.927494000	0.403608000
H	2.068180000	0.547271000	1.668068000
S	-1.870903000	-0.927538000	0.404013000
H	-2.064390000	-0.547736000	1.668944000
S	-1.919337000	0.916787000	-0.488385000
H	-0.629290000	1.223450000	-0.310841000

Conformer 2pe

S	1.718145000	0.322903000	1.001720000
H	0.626723000	1.087751000	0.857917000
S	1.753390000	-0.425724000	-0.907079000
H	2.549762000	0.495910000	-1.453250000
S	-1.833594000	-0.969912000	0.283755000
H	-0.727423000	-0.978862000	1.036408000
S	-1.732405000	0.984572000	-0.319731000
H	-0.937646000	0.805784000	-1.379716000

Conformer 2pf

S	1.755101000	0.610632000	-0.822614000
H	0.794371000	1.451489000	-0.421405000
S	1.754508000	-0.610685000	0.822872000
H	0.792960000	-1.450500000	0.421475000
S	-1.754510000	-0.823101000	-0.610451000
H	-0.793680000	-0.422073000	-1.451185000
S	-1.755053000	0.823089000	0.610186000
H	-0.794394000	0.422118000	1.451227000

Optimized conformers for the $(H_2S_2)_3$ trimer (Fig. 2B)

Conformer 3pa

H	0.937237000	0.720969000	-1.325671000
H	-0.431834000	1.848998000	1.120976000
S	0.897408000	1.739928000	1.042044000
S	1.076589000	2.006344000	-0.979304000
H	-1.698955000	-0.865847000	1.036315000
H	-4.298999000	-1.514520000	-0.469602000
S	-2.015891000	-0.314699000	-0.137503000
S	-4.057771000	-0.317868000	0.068866000
S	3.088324000	-1.232746000	0.039122000
H	3.364193000	-2.022829000	1.078732000
S	1.075125000	-1.602862000	-0.064855000
H	1.107816000	-2.616328000	-0.934655000

Conformer 3pb

H	0.803369000	1.443345000	-1.184715000
H	-0.767761000	1.525882000	1.384005000
S	0.082315000	2.506331000	1.061717000
S	-0.133322000	2.374176000	-0.970151000
H	-2.611575000	0.253445000	-1.084713000
H	-2.751740000	-2.791685000	-0.656113000
S	-1.788289000	-0.405854000	-0.267508000
S	-3.054555000	-1.917792000	0.305708000
S	3.464686000	-1.432940000	-0.005585000
H	3.385657000	-2.389828000	0.920851000
S	1.484030000	-0.894164000	-0.023692000
H	1.064217000	-1.717265000	-0.987130000

Conformer 3pc

H	-0.906690000	-1.425840000	1.355992000
H	-1.709319000	0.003671000	-1.185875000
S	-2.158118000	-1.223246000	-0.897140000
S	-2.167040000	-1.028525000	1.145517000
H	-0.683156000	1.227981000	1.368504000
H	-1.102180000	3.218466000	-0.920996000
S	0.258576000	2.101962000	0.997237000
S	-0.248546000	2.193603000	-0.989149000
S	3.119871000	-1.035162000	0.229164000
H	3.618058000	-0.249414000	-0.727288000
S	1.168162000	-1.047891000	-0.406024000
H	1.216808000	-2.146725000	-1.164007000

Conformer 3pd

H	-0.973820000	0.397375000	-1.213008000
H	0.947891000	0.540126000	1.130459000
S	-0.001408000	-0.403445000	1.038826000
S	-0.017394000	-0.520890000	-1.009039000
H	3.837702000	1.548069000	1.040200000
H	2.580729000	-1.232658000	0.592100000
S	3.177495000	1.194560000	-0.065365000
S	3.660797000	-0.797037000	-0.067081000
S	-3.683135000	-0.766720000	0.122981000
H	-2.638256000	-1.279955000	-0.536922000
S	-3.220841000	1.211072000	-0.140388000
H	-2.402471000	1.346379000	0.908206000

Conformer 3pe

H	-0.749762000	-1.578738000	1.238359000
H	-1.842249000	0.109578000	-1.047706000
S	-2.024912000	-1.214478000	-0.979077000
S	-2.064033000	-1.395356000	1.064356000
H	-1.003985000	1.095190000	1.290330000
H	0.410894000	1.472711000	-1.368336000
S	-0.087811000	2.051600000	1.102987000
S	-0.436599000	2.391378000	-0.889835000
S	3.219018000	-0.881376000	0.239474000
H	3.688010000	0.046271000	-0.597042000
S	1.276215000	-0.905887000	-0.424337000
H	1.387034000	-1.879115000	-1.332677000

Conformer 3pf

H	3.808763000	-0.896701000	-1.271320000
H	0.812892000	-0.697641000	-0.759537000
S	1.590647000	-1.548279000	-0.076491000
S	3.306004000	-0.424513000	-0.128872000
H	0.913420000	0.666536000	1.259292000
H	-1.160918000	1.292669000	-0.969231000
S	0.256718000	1.827814000	1.131509000
S	0.080307000	1.791391000	-0.913315000
S	-3.219008000	-0.254555000	-0.569315000
H	-4.096648000	0.087609000	0.376555000
S	-1.957414000	-1.395236000	0.576877000
H	-1.193591000	-0.398422000	1.037949000

Conformer 3pg

H	-0.023615000	-1.191705000	-1.411010000
H	-0.830094000	-3.366004000	0.580886000
S	-1.092626000	-2.071293000	0.779890000
S	-1.301704000	-1.513810000	-1.184147000
H	1.320993000	-1.029725000	1.131916000
H	1.381658000	0.988896000	-1.132380000
S	2.290129000	-0.111272000	1.037256000
S	2.320668000	0.042508000	-1.013251000
S	-1.004971000	2.100590000	-0.789561000
H	-0.705548000	3.386533000	-0.585798000
S	-1.281672000	1.554509000	1.169104000
H	-0.020570000	1.192265000	1.427737000

Conformer 3ph

H	2.992516000	0.596160000	0.357395000
H	0.806435000	-1.057158000	-0.886832000
S	1.610101000	-1.579204000	0.045497000
S	3.288282000	-0.482103000	-0.376732000
H	0.833422000	0.468713000	1.263796000
H	-1.149973000	1.390994000	-0.889299000
S	0.380738000	1.731335000	1.177647000
S	0.135421000	1.763464000	-0.860554000
S	-3.250645000	-0.150902000	-0.600602000
H	-4.132528000	0.194834000	0.339942000
S	-2.045355000	-1.357211000	0.539343000
H	-1.246534000	-0.399596000	1.021409000

Conformer 3pi

H	0.965470000	0.418463000	1.177622000
H	-0.964622000	0.418070000	-1.176833000
S	-0.007936000	-0.511154000	-1.025618000
S	0.008736000	-0.510827000	1.026865000
H	-2.370088000	1.294136000	0.984141000
H	-2.652194000	-1.254871000	-0.596623000
S	-3.174592000	1.229140000	-0.081779000
S	-3.689519000	-0.746607000	0.078621000
S	3.688462000	-0.747001000	-0.079326000
H	2.649144000	-1.254492000	0.593434000
S	3.174853000	1.229149000	0.081487000
H	2.372226000	1.295483000	-0.985735000

Conformer 3pj

H	1.348749000	0.466605000	-1.061410000
H	3.124111000	0.378719000	1.467653000
S	2.495999000	-0.688226000	0.967448000
S	2.532766000	-0.156161000	-1.013296000
H	0.280279000	0.732359000	1.055092000
H	-1.845544000	1.100258000	-1.072147000
S	-0.583176000	1.757086000	1.097947000
S	-0.858893000	1.992799000	-0.920522000
S	-0.856726000	-1.700244000	-0.457601000
H	-0.521317000	-2.545851000	0.520084000
S	-2.731384000	-1.203369000	0.208568000
H	-2.363665000	-0.162246000	0.970021000

Conformer 3pk

H	0.439376000	1.896167000	0.584094000
H	-2.544939000	2.261802000	1.128931000
S	-2.083822000	1.412669000	0.206674000
S	-0.393355000	2.457636000	-0.303739000
H	-1.556405000	-0.977324000	1.201435000
H	0.303289000	-1.375099000	-1.198046000
S	-1.136115000	-2.187086000	0.810145000
S	-0.977817000	-1.759347000	-1.190519000
S	2.540035000	-0.023096000	-0.815398000
H	1.619492000	0.866035000	-1.210418000
S	2.089068000	-0.008655000	1.187616000
H	1.131274000	-0.945519000	1.177530000

Conformer 3pl

H	0.023197000	-1.172947000	-1.296212000
H	-1.617325000	-0.971181000	1.279345000
S	-1.364390000	-2.142281000	0.683352000
S	-1.287849000	-1.433232000	-1.240590000
H	1.166891000	-1.303874000	0.978389000
H	1.511048000	0.960289000	-1.029998000
S	2.171536000	-0.423061000	1.070622000
S	2.406426000	-0.029673000	-0.934078000
S	-0.863379000	2.182037000	-0.803445000
H	-0.470710000	3.448378000	-0.636885000
S	-1.108165000	1.709568000	1.180562000
H	0.120032000	1.225609000	1.402596000

Conformer 3pm

H	0.405981000	0.464877000	-1.210957000
H	-1.191837000	1.223219000	1.274177000
S	0.055699000	1.659428000	1.055515000
S	-0.033915000	1.712750000	-0.990399000
H	-2.404081000	0.773150000	-0.726985000
H	-2.103720000	-2.234681000	-0.988407000
S	-3.223770000	-0.065826000	-0.074602000
S	-1.882801000	-1.597496000	0.163642000
S	3.344569000	-0.167607000	-0.093497000
H	4.000609000	-0.640859000	0.968118000
S	1.761225000	-1.469294000	-0.062850000
H	0.956932000	-0.736981000	0.719130000

Conformer 3pn

H	0.087808000	-1.417243000	0.558775000
H	2.614731000	-0.002228000	-0.473073000
S	2.666111000	-1.088151000	0.310506000
S	0.923895000	-1.953006000	-0.337407000
H	1.299816000	0.920145000	1.313000000
H	-0.104988000	1.032695000	-1.361300000
S	0.491813000	1.940386000	0.988117000
S	0.838497000	1.922703000	-1.033541000
S	-2.355738000	-0.375474000	-0.991324000
H	-3.366994000	0.475211000	-1.182833000
S	-2.493355000	-0.539024000	1.050806000
H	-1.669949000	0.472474000	1.350927000

Conformer 3po

H	-2.821151000	0.780021000	-0.738347000
H	-1.043281000	-1.005648000	0.886377000
S	-1.811650000	-1.513067000	-0.084113000
S	-3.347696000	-0.164281000	0.048909000
H	-0.340546000	0.281218000	-1.157053000
H	1.195388000	1.300276000	1.244787000
S	-0.032264000	1.581404000	-1.015803000
S	-0.085895000	1.627921000	1.032788000
S	1.929777000	-1.540487000	0.177166000
H	2.222152000	-2.221829000	-0.932953000
S	3.245127000	0.011982000	-0.067150000
H	2.429057000	0.810398000	-0.771570000

Conformer 3pp

H	-1.224432000	1.541656000	-0.745852000
H	1.454461000	1.337933000	0.743562000
S	1.197792000	2.300060000	-0.152742000
S	-0.826272000	2.452090000	0.152714000
H	1.716963000	-0.083318000	-1.197025000
H	0.485044000	-1.456733000	1.227052000
S	1.907973000	-1.386919000	-0.951532000
S	1.807434000	-1.292109000	1.097524000
S	-2.100823000	-1.080130000	0.951612000
H	-1.711740000	0.178616000	1.197015000
S	-1.987033000	-1.002408000	-1.097440000
H	-0.705437000	-1.367515000	-1.226922000

Optimized conformers for the $H_2S_2.H_2O$ complex (Fig. 3A)

Conformer pwa

O	-3.068095000	0.207807000	0.095192000
H	-3.171264000	0.162280000	-0.856879000
H	-3.566108000	-0.542820000	0.422622000
S	-0.080196000	-0.257067000	-0.089316000
H	-0.524383000	0.799681000	0.588075000
S	1.928663000	0.157778000	-0.035937000
H	2.231038000	-0.492980000	1.088699000

Conformer pwb

O	-2.447988000	-0.081122000	0.091244000
H	-1.821486000	0.623804000	-0.101760000
H	-3.158828000	0.044466000	-0.538797000
S	0.703298000	1.022309000	-0.083972000
H	0.743394000	1.276428000	1.225961000
S	0.816658000	-1.024804000	-0.002510000
H	-0.498460000	-1.255801000	0.068355000

Optimized conformers for the $2H_2O.H_2S_2$ complex (Fig. 3B)

Conformer 2wpa

O	3.153141000	-0.597005000	-0.004238000
H	2.386998000	-1.154872000	-0.166589000
H	3.846077000	-0.963101000	-0.555590000
O	-3.628767000	-0.337404000	0.009078000
H	-2.677463000	-0.376797000	-0.126693000
H	-3.944923000	0.229354000	-0.695319000
S	-0.189942000	-0.689264000	-0.009881000
H	-0.263798000	-0.901872000	1.306767000
S	0.363381000	1.287458000	0.021932000
H	1.683099000	1.071454000	0.005890000

Conformer 2wpb

O	1.715016000	1.598657000	-0.656598000
H	2.099820000	0.820530000	-0.235209000
H	0.925707000	1.764577000	-0.138245000
O	2.353420000	-0.976593000	0.561085000
H	1.453884000	-1.285596000	0.411646000
H	2.534798000	-1.166332000	1.482668000
S	-1.431044000	0.590159000	0.638493000
H	-2.227610000	1.241459000	-0.211035000
S	-0.796251000	-0.874440000	-0.652465000
H	-1.697373000	-1.802651000	-0.322176000

Conformer 2wpc

O	-1.795197000	1.474662000	0.730833000
H	-2.083555000	0.728615000	0.190425000
H	-1.080257000	1.854057000	0.217593000
O	-2.129005000	-0.985700000	-0.778921000
H	-1.342710000	-1.314551000	-0.329538000
H	-2.809492000	-1.636764000	-0.601213000

S	1.320163000	0.579750000	-0.719154000
H	2.206821000	1.292748000	-0.021954000
S	0.852508000	-0.774891000	0.751416000
H	1.740064000	-1.713532000	0.413191000

Conformer 2wpd

O	2.260181000	1.401054000	-0.059586000
H	1.866224000	0.920598000	0.675862000
H	3.192483000	1.454031000	0.154754000
O	-2.259054000	1.404554000	0.052604000
H	-3.194292000	1.438346000	-0.152775000
H	-1.864706000	0.920471000	-0.680277000
S	0.022987000	-0.850251000	1.030080000
H	-0.925161000	0.076326000	1.213729000
S	-0.023597000	-0.857291000	-1.026231000
H	0.926197000	0.066044000	-1.217033000

Conformer 2wpe

O	-1.617716000	1.335531000	0.720617000
H	-2.243762000	2.061035000	0.750054000
H	-0.944909000	1.602153000	0.084421000
O	-2.250899000	-1.142408000	-0.745256000
H	-1.476089000	-1.658248000	-0.516377000
H	-2.158419000	-0.347779000	-0.207457000
S	1.034152000	-0.813399000	0.733885000
H	0.080019000	-0.183351000	1.425261000
S	1.187859000	0.542489000	-0.800482000
H	2.139895000	1.315770000	-0.273230000

Conformer 2wpf

O	-1.422698000	-0.269166000	0.129680000
H	-2.365502000	-0.071691000	0.058662000
H	-0.973430000	0.564134000	-0.028949000
O	-4.248896000	0.165227000	-0.063940000
H	-4.662155000	-0.311521000	-0.785884000
H	-4.740500000	-0.098649000	0.715749000
S	1.802647000	-1.002111000	-0.017942000
H	0.487672000	-1.229047000	0.077105000
S	1.688960000	1.044773000	-0.093206000
H	1.760945000	1.295677000	1.215769000

Conformer 2wpg

O	2.012922000	-1.417857000	-0.293027000
H	2.216856000	-0.477908000	-0.401646000
H	2.035208000	-1.780678000	-1.179023000
O	2.038897000	1.392103000	-0.029930000
H	1.167454000	1.344736000	0.381277000
H	2.013858000	2.173797000	-0.583402000
S	-0.754884000	-0.135162000	1.063018000
H	0.244831000	-0.936016000	0.657278000
S	-1.596864000	0.179861000	-0.783083000
H	-2.464795000	-0.833086000	-0.769780000

Conformer 2wph

O	2.064133000	-1.213002000	-0.665946000
H	2.890351000	-1.675451000	-0.523309000
H	2.249360000	-0.287433000	-0.448335000
O	1.962325000	1.444335000	0.277494000
H	1.110715000	1.233066000	0.679003000
H	1.783292000	2.189112000	-0.299076000
S	-0.758897000	-0.455578000	0.973731000
H	0.258946000	-1.087357000	0.367888000
S	-1.620469000	0.357529000	-0.702481000
H	-2.434468000	-0.653831000	-1.008543000

Conformer 2wpi

O	2.040173000	-1.411786000	-0.266805000
H	2.214346000	-0.465256000	-0.375024000
H	2.061901000	-1.770032000	-1.154796000
O	1.959150000	1.408094000	-0.181058000
H	1.151278000	1.345277000	0.343025000
H	2.526409000	2.009253000	0.304062000
S	-0.751434000	-0.125890000	1.064065000
H	0.239779000	-0.940609000	0.666509000
S	-1.604919000	0.168545000	-0.780709000
H	-2.486641000	-0.831576000	-0.734568000

Conformer 2wpj

O	2.075345000	-1.258864000	-0.509527000
H	2.132418000	-0.296982000	-0.429938000
H	2.108095000	-1.431328000	-1.451076000
O	1.677844000	1.479462000	0.227477000
H	1.008615000	1.147380000	0.840244000
H	2.258457000	2.026493000	0.759149000

S	-0.828129000	-0.462078000	0.995640000
H	0.170382000	-1.221655000	0.521510000
S	-1.488357000	0.257634000	-0.811784000
H	-0.639711000	1.282419000	-0.925191000

Conformer 2wpk

O	2.003491000	1.424091000	0.276744000
H	2.224978000	0.499564000	0.081396000
H	2.519010000	1.938346000	-0.345510000
O	2.122622000	-1.309123000	-0.263035000
H	1.166594000	-1.419702000	-0.168299000
H	2.508217000	-1.958950000	0.326502000
S	-1.201394000	-1.024664000	0.059457000
H	-1.330109000	-1.106111000	1.385979000
S	-1.304817000	1.014967000	-0.147721000
H	0.001788000	1.282254000	0.022479000

Conformer 2wpl

O	2.136614000	-1.316708000	-0.146267000
H	2.411950000	-1.709914000	-0.976005000
H	1.174478000	-1.413501000	-0.129628000
O	1.983792000	1.453637000	0.151499000
H	2.214904000	0.515055000	0.063293000
H	2.435920000	1.748401000	0.942606000
S	-1.312131000	0.995738000	-0.205945000
H	-0.010590000	1.289658000	-0.042774000
S	-1.182161000	-1.026315000	0.121440000
H	-1.281228000	-1.035905000	1.452733000

Optimized conformers for the $2H_2S_2.H_2O$ complex (Fig. 3C)

Conformer 2pwa

S	-1.042711000	1.341740000	-0.522038000
H	0.271377000	1.416546000	-0.280270000
S	-1.308744000	-0.558646000	0.202057000
H	-1.522128000	-0.264112000	1.487375000
S	2.635347000	0.678075000	0.508945000
H	2.681218000	0.222128000	1.762669000
S	2.491829000	-1.115502000	-0.472464000
H	1.162604000	-1.241794000	-0.399542000
O	-4.747922000	-0.552659000	0.303397000
H	-3.815689000	-0.594791000	0.071244000
H	-5.205542000	-0.647371000	-0.532673000

Conformer 2pwb

S	-1.672437000	-1.234671000	-0.173723000
H	-2.799973000	-1.599131000	-0.789182000
S	-2.130750000	0.752305000	0.048024000
H	-2.574903000	0.701228000	1.305411000
S	1.547654000	-0.490462000	1.089349000
H	1.775710000	-1.790845000	1.288498000
S	1.962313000	-0.445887000	-0.918832000
H	0.728577000	-0.720474000	-1.358011000
O	0.775261000	2.724825000	-0.084832000
H	1.368561000	2.123133000	-0.541569000
H	-0.008531000	2.186919000	0.056417000

Conformer 2pwc

S	0.982168000	-0.836667000	-1.013822000
H	-0.270849000	-1.304177000	-0.918938000
S	1.144780000	-0.234012000	0.942267000
H	1.717456000	-1.336458000	1.433052000
S	-2.107070000	1.305804000	-0.222439000
H	-1.032745000	1.062908000	-0.982080000
S	-2.553702000	-0.638690000	0.241244000
H	-1.772912000	-0.751934000	1.320326000
O	4.268110000	0.794172000	-0.025752000
H	3.385153000	0.694186000	0.342310000
H	4.370192000	1.739145000	-0.144660000

Conformer 2pwd

S	3.480224000	-0.756336000	-0.546587000
H	4.787478000	-0.779130000	-0.279885000
S	2.981152000	0.778722000	0.719449000
H	3.091388000	1.789697000	-0.145433000
S	-3.370037000	0.843486000	-0.491842000
H	-2.070482000	0.979754000	-0.780403000
S	-3.186630000	-0.868981000	0.623394000
H	-3.327170000	-1.762075000	-0.358762000
O	-0.120668000	0.008543000	-0.442066000
H	-0.642997000	-0.524730000	0.164911000
H	0.651778000	0.277900000	0.065472000

Conformer 2pwe

S	-1.606830000	-0.812316000	-0.952847000
H	-1.938648000	-2.060369000	-0.615580000
S	-2.130145000	0.109895000	0.801817000

H	-0.947020000	-0.021248000	1.413701000
S	1.916488000	-0.208826000	-0.878869000
H	3.196686000	0.172439000	-0.856041000
S	1.679305000	-0.446425000	1.146030000
H	1.907725000	-1.760312000	1.201733000
O	0.026780000	2.655852000	-0.293270000
H	0.592967000	1.958055000	-0.634651000
H	-0.767038000	2.187368000	-0.021111000

Conformer 2pwf

S	2.108670000	1.146610000	-0.089974000
H	1.040750000	1.934764000	-0.080168000
S	1.865169000	0.311016000	1.774585000
H	1.052212000	-0.693323000	1.419973000
S	-0.283860000	-1.745281000	-0.412394000
H	0.793543000	-1.143300000	-0.917917000
S	-1.511801000	-0.098451000	-0.335192000
H	-1.243198000	0.286560000	0.912860000
O	2.796920000	-2.075684000	-0.197144000
H	3.626539000	-2.577574000	-0.330745000
H	3.125376000	-1.646549000	0.580222000

Conformer 2pwg

S	-0.996432000	-0.623860000	1.049676000
H	-1.807188000	-1.588582000	1.494025000
S	-1.153469000	-1.010277000	-0.960910000
H	-2.181155000	-0.185628000	-1.192713000
S	1.671670000	1.315327000	-0.161114000
H	2.221611000	1.880133000	0.916237000
S	2.589750000	-0.510530000	-0.027840000
H	1.638207000	-1.121993000	0.685663000
O	-3.434160000	1.355379000	-0.090920000
H	-2.790597000	1.132432000	0.589271000
H	-3.391905000	2.310039000	-0.162119000

Conformer 2pwh

S	1.608879000	1.295772000	0.065918000
H	2.438789000	2.011085000	-0.697860000
S	2.558101000	-0.513456000	-0.111131000
H	3.334127000	-0.418215000	0.970146000
S	-1.041753000	-0.850058000	1.053571000
H	-1.979431000	0.078779000	1.270984000
S	-1.209651000	-0.900960000	-0.990062000
H	-0.307201000	0.051750000	-1.258404000

O	-3.355290000	1.438136000	0.024236000
H	-4.298566000	1.443433000	-0.143756000
H	-2.994617000	0.827305000	-0.627721000

Conformer 2pwi

S	1.941753000	-0.119369000	-0.951903000
H	0.682939000	-0.437836000	-1.277368000
S	1.836285000	-0.632978000	1.032304000
H	2.138174000	-1.927747000	0.913033000
S	-1.880283000	-0.805773000	-0.900202000
H	-2.220006000	-2.027196000	-0.482598000
S	-1.961322000	0.162325000	0.907404000
H	-0.712384000	-0.111784000	1.303596000
O	0.121404000	2.802388000	-0.185112000
H	-0.625702000	2.258459000	0.078064000
H	0.782813000	2.159726000	-0.455494000

Conformer 2pwj

S	2.664855000	-0.462374000	-0.463113000
H	2.876890000	-1.616117000	0.172305000
S	1.380997000	0.365783000	0.905260000
H	2.284047000	1.049958000	1.613283000
S	-2.538550000	-0.048259000	0.517492000
H	-2.064310000	1.098277000	0.011531000
S	-1.221936000	-1.300318000	-0.433250000
H	-1.926759000	-1.523474000	-1.544803000
O	-0.660113000	2.464308000	-0.807586000
H	-0.527313000	2.454995000	-1.756925000
H	0.072493000	1.944572000	-0.456911000

Conformer 2pwk

S	2.496664000	-0.457044000	-0.507614000
H	2.596130000	-1.717301000	-0.080943000
S	1.376616000	0.261563000	1.052024000
H	2.376850000	0.737436000	1.798248000
S	-1.333098000	-1.043841000	-0.771498000
H	-0.824246000	0.057298000	-1.338638000
S	-2.410974000	-0.093989000	0.690962000
H	-1.466492000	-0.081514000	1.636592000
O	-0.456536000	2.258410000	-1.059110000
H	-1.287495000	2.249887000	-0.576697000
H	0.190203000	2.019872000	-0.387676000

Conformer 2pwl

S	1.581635000	-0.799951000	1.049344000
H	2.007322000	0.466904000	1.098905000
S	1.272873000	-0.892209000	-0.977980000
H	2.511729000	-1.234220000	-1.341194000
S	-2.252130000	-0.838666000	-0.107920000
H	-2.986944000	-0.928710000	1.002529000
S	-1.654779000	1.110942000	0.088512000
H	-0.531597000	0.882868000	0.775806000
O	1.604535000	2.327231000	-0.124545000
H	1.351605000	1.723928000	-0.830750000
H	1.650011000	3.189524000	-0.540221000

Conformer 2pwm

S	2.592590000	-0.580696000	0.008747000
H	1.577830000	-1.108106000	0.703153000
S	1.812218000	1.302955000	-0.200106000
H	2.394365000	1.865497000	0.861892000
S	-1.117343000	-0.938111000	-0.943403000
H	-2.154360000	-0.142328000	-1.228080000
S	-1.106283000	-0.604006000	1.081653000
H	-0.287437000	0.459119000	1.069621000
O	-3.592717000	1.249534000	-0.151494000
H	-3.159893000	0.830716000	0.599467000
H	-4.527668000	1.216570000	0.055636000

Conformer 2pwn

S	1.711445000	-1.218590000	-0.286372000
H	2.839055000	-1.741006000	0.202562000
S	2.062298000	0.714875000	0.305538000
H	2.599232000	1.170768000	-0.828450000
S	-1.785208000	-0.479121000	-0.983162000
H	-1.470320000	0.819821000	-1.070181000
S	-1.775619000	-0.599271000	1.064503000
H	-0.511065000	-1.009225000	1.210832000
O	-0.699388000	2.655862000	-0.219681000
H	-1.281093000	2.737948000	0.538810000
H	0.012651000	2.088505000	0.095762000

Conformer 2pwo

S	1.425955000	1.005125000	-0.957116000
H	0.708216000	2.129559000	-0.913858000
S	1.561604000	0.676601000	1.063227000

H	0.445107000	-0.062779000	1.186068000
S	-1.539019000	-1.094397000	0.108721000
H	-0.568189000	-0.978838000	-0.803340000
S	-2.334620000	0.786561000	-0.073055000
H	-1.576467000	1.397872000	0.842613000
O	1.406272000	-2.438552000	-0.295983000
H	2.023343000	-3.156225000	-0.447349000
H	1.895095000	-1.803404000	0.235291000

Conformer 2pwp

S	1.551605000	1.075963000	0.120351000
H	0.538392000	0.899808000	-0.734203000
S	2.309724000	-0.828610000	0.060999000
H	3.155901000	-0.673874000	-0.959396000
S	-1.670487000	-0.640252000	1.044731000
H	-0.497902000	-0.021268000	1.252496000
S	-1.418962000	-1.008828000	-0.957238000
H	-0.775836000	-2.173270000	-0.847331000
O	-1.365886000	2.432771000	-0.337831000
H	-1.992811000	3.137708000	-0.507063000
H	-1.850733000	1.796360000	0.196657000

Conformer 2pwq

S	-2.226936000	-0.899720000	0.335452000
H	-3.499631000	-0.533570000	0.504037000
S	-1.632014000	0.713379000	-0.785393000
H	-1.099952000	1.447331000	0.198560000
S	1.421214000	-1.266718000	0.621935000
H	1.523384000	-2.393816000	-0.085423000
S	2.110530000	0.025649000	-0.813568000
H	0.916327000	0.320010000	-1.346746000
O	0.626968000	2.404811000	1.068088000
H	1.326414000	1.873113000	0.671778000
H	1.053009000	2.887017000	1.778256000

Conformer 2pwr

S	1.773666000	0.818691000	-0.569762000
H	0.574829000	0.453971000	-1.046472000
S	2.268346000	-0.951399000	0.345375000
H	2.862464000	-1.540023000	-0.694647000
S	-1.979283000	-0.042739000	-0.993646000
H	-1.784052000	1.130078000	-0.374069000
S	-1.685834000	-1.239130000	0.651565000
H	-0.368659000	-1.424247000	0.520150000

O	-0.790598000	2.456053000	0.980043000
H	0.083525000	2.055142000	0.933640000
H	-1.073640000	2.309866000	1.884553000

Conformer 2pws

S	1.111872000	-0.773726000	1.060479000
H	0.259621000	0.260297000	1.150484000
S	1.100272000	-0.942704000	-0.986733000
H	2.109731000	-0.096486000	-1.221699000
S	-2.596154000	-0.501578000	-0.041602000
H	-1.690397000	-1.134267000	0.712294000
S	-1.740570000	1.358587000	0.000999000
H	-0.894613000	1.190676000	-1.021547000
O	3.362913000	1.382476000	-0.112281000
H	3.029337000	0.893363000	0.646539000
H	4.276315000	1.577353000	0.101898000

Conformer 2pwt

S	-2.242338000	0.330620000	0.598104000
H	-1.330345000	1.259559000	0.280849000
S	-1.647675000	-1.133806000	-0.709339000
H	-0.790640000	-1.764818000	0.100334000
S	1.725284000	-0.691725000	1.065142000
H	2.274478000	-1.896660000	0.897100000
S	1.952801000	-0.022332000	-0.862018000
H	0.722182000	-0.345271000	-1.291392000
O	0.140329000	2.684454000	-0.177371000
H	0.902518000	2.122362000	-0.358715000
H	0.490035000	3.425084000	0.320574000

Conformer 2pwu

S	-2.401103000	-0.792904000	-0.361649000
H	-1.310966000	-1.564020000	-0.321222000
S	-1.678248000	0.753822000	0.775073000
H	-1.052551000	1.437411000	-0.189340000
S	1.455806000	-1.221156000	-0.630762000
H	1.079766000	-0.217237000	-1.430184000
S	2.062036000	-0.081305000	0.965603000
H	0.860053000	0.070843000	1.534745000
O	0.839439000	2.121613000	-1.181954000
H	1.465692000	1.884907000	-0.487952000
H	1.226639000	2.879889000	-1.622648000

Conformer 2pwv

S	-2.196482000	0.636398000	0.410821000
H	-1.158247000	1.344546000	-0.049790000
S	-1.767389000	-1.155938000	-0.489704000
H	-0.987315000	-1.661431000	0.471752000
S	1.593455000	-0.504994000	1.181412000
H	1.141789000	0.748470000	1.288787000
S	1.938079000	-0.500692000	-0.841658000
H	0.694228000	-0.824421000	-1.227427000
O	0.644670000	2.455049000	-0.382577000
H	0.842748000	3.316825000	-0.752820000
H	1.226825000	1.839234000	-0.843821000

Optimized conformers for the H_2S_2.ethane complex

Conformer 1a

C	-2.130432000	0.293267000	0.027784000
H	-1.361698000	-0.470131000	-0.074276000
H	-1.987776000	1.012906000	-0.775673000
H	-1.957700000	0.811906000	0.968680000
C	-3.520666000	-0.317573000	-0.018901000
H	-3.690664000	-0.835876000	-0.960076000
H	-3.661275000	-1.037711000	0.784303000
H	-4.290517000	0.444380000	0.082334000
S	1.254234000	1.004030000	0.000358000
H	2.513400000	1.445940000	0.028223000
S	1.663249000	-1.002433000	-0.083738000
H	1.663089000	-1.251124000	1.227270000

Conformer 1b

C	-2.281435000	0.303453000	0.686457000
H	-2.262693000	1.384941000	0.568846000
H	-3.145452000	0.050941000	1.297992000
H	-1.390458000	0.012483000	1.239360000
C	-2.337559000	-0.396322000	-0.660456000
H	-3.237699000	-0.123902000	-1.207880000
H	-1.481547000	-0.127338000	-1.275514000
H	-2.333651000	-1.477648000	-0.541725000
S	1.288945000	-0.997382000	0.054205000
H	1.843583000	-1.027022000	1.267654000
S	1.054303000	1.032043000	-0.106141000
H	2.229907000	1.310192000	-0.673760000

Optimized conformers for the H_2S_2.acetamide complex

Conformer 2a

C	1.549906000	-0.946652000	-1.041552000
H	1.100425000	-1.865487000	-0.673668000
H	0.808504000	-0.404055000	-1.626353000
H	2.393174000	-1.176604000	-1.683077000
C	2.019663000	-0.052503000	0.076987000
O	2.963784000	0.707359000	-0.042104000
H	1.503046000	0.511939000	1.959880000
H	0.443221000	-0.667365000	1.265370000
N	1.304955000	-0.151562000	1.231160000
S	-2.050535000	-0.787916000	0.275679000
H	-1.716675000	-1.434445000	-0.843947000
S	-1.460216000	1.096548000	-0.281147000
H	-2.622048000	1.494892000	-0.804627000

Conformer 2b

C	1.452033000	0.871191000	0.983377000
H	0.583542000	1.354761000	0.541874000
H	1.112192000	0.321258000	1.856550000
H	2.172271000	1.624881000	1.288138000
C	2.002196000	-0.106659000	-0.015490000
O	1.344752000	-1.048401000	-0.437075000
H	3.667807000	-0.512614000	-1.110848000
H	3.813928000	0.885302000	-0.096752000
N	3.271353000	0.113137000	-0.431928000
S	-1.855317000	-0.956503000	0.364392000
H	-0.551306000	-1.108020000	0.066013000
S	-2.071767000	0.944289000	-0.376079000
H	-2.347943000	0.637900000	-1.645214000

Conformer 2c

C	-3.460543000	-0.087205000	-0.057759000
H	-3.864437000	-0.390337000	0.904034000
H	-3.903794000	0.859618000	-0.352120000
H	-3.725971000	-0.851158000	-0.782753000
C	-1.961546000	-0.037823000	0.051935000
O	-1.314558000	-1.031583000	0.361233000
H	-0.375184000	1.240655000	-0.129344000
H	-1.925925000	1.954501000	-0.457716000
N	-1.380094000	1.152687000	-0.206638000
S	1.903828000	-1.067731000	-0.194358000
H	0.579322000	-1.153367000	0.049620000

S	2.075420000	0.960569000	0.067484000
H	2.257675000	0.988707000	1.389815000

Optimized conformers for the H_2S_2.N-methylacetamide complex

Conformer 3a

C	1.199855000	1.891816000	-0.293033000
H	0.630528000	1.961313000	-1.216511000
H	0.578137000	2.217598000	0.538165000
H	2.059290000	2.553568000	-0.346626000
C	1.682473000	0.495746000	0.000231000
O	2.468169000	0.250570000	0.903341000
H	0.428789000	-0.251155000	-1.421790000
N	1.183290000	-0.479517000	-0.799059000
C	1.472449000	-1.865682000	-0.517989000
H	0.987219000	-2.483739000	-1.266825000
H	2.544836000	-2.036994000	-0.550054000
H	1.113676000	-2.146803000	0.471462000
S	-2.263605000	0.140987000	-0.709024000
H	-2.198926000	1.472240000	-0.627622000
S	-1.351643000	-0.310416000	1.073315000
H	-2.456622000	-0.354371000	1.822565000

Conformer 3b

C	-1.254214000	1.872743000	-0.184597000
H	-0.608286000	2.115767000	0.657906000
H	-0.679598000	1.959072000	-1.103336000
H	-2.073698000	2.583844000	-0.195121000
C	-1.814569000	0.490441000	0.024833000
O	-2.750415000	0.262524000	0.776632000
H	-0.392255000	-0.279130000	-1.230457000
N	-1.179900000	-0.503356000	-0.646147000
C	-1.582540000	-1.880091000	-0.478003000
H	-2.597829000	-2.032998000	-0.836549000
H	-0.902614000	-2.513580000	-1.038807000
H	-1.554338000	-2.161768000	0.572942000
S	2.219517000	0.174532000	-0.816376000
H	2.115241000	1.501858000	-0.714562000
S	1.804356000	-0.311753000	1.131512000
H	0.481954000	-0.452794000	0.982392000

Conformer 3c

C	-0.817909000	1.353915000	-0.943580000
H	0.042730000	1.601250000	-0.325961000
H	-0.446595000	1.047721000	-1.917833000
H	-1.446551000	2.233032000	-1.057283000
C	-1.533389000	0.194221000	-0.312552000
O	-0.995961000	-0.897574000	-0.144150000
H	-3.219746000	1.309459000	-0.071947000
N	-2.808551000	0.406562000	0.072665000
C	-3.572782000	-0.643496000	0.705987000
H	-4.567606000	-0.270110000	0.924630000
H	-3.647206000	-1.507531000	0.050697000
H	-3.094618000	-0.960865000	1.629369000
S	2.257231000	-0.890870000	-0.552324000
H	0.916359000	-0.987403000	-0.456587000
S	2.496425000	0.670122000	0.757191000
H	2.576765000	-0.026762000	1.892454000

Conformer 3d

C	-2.037585000	-1.701303000	0.145532000
H	-1.164662000	-2.349013000	0.136323000
H	-2.663935000	-1.991544000	0.983876000
H	-2.589103000	-1.832395000	-0.781725000
C	-1.566814000	-0.291904000	0.362801000
O	-1.033720000	0.059849000	1.410795000
H	-2.135603000	0.222650000	-1.519737000
N	-1.769736000	0.573788000	-0.654332000
C	-1.277765000	1.930015000	-0.585413000
H	-1.710617000	2.505591000	-1.397325000
H	-1.567899000	2.372312000	0.363195000
H	-0.190656000	1.964607000	-0.655205000
S	2.118514000	0.423794000	0.702745000
H	0.899378000	0.443633000	1.266222000
S	1.617132000	-0.775614000	-0.882427000
H	1.303664000	0.177120000	-1.764267000

Optimized conformers for the H_2S_2.methylamine complex

Conformer 4a

C	2.319191000	0.146700000	0.646878000
H	3.235867000	-0.301941000	1.021805000
H	2.403725000	1.221378000	0.790234000
H	1.489795000	-0.219027000	1.260426000
N	2.193260000	-0.134919000	-0.775520000

H	2.108798000	-1.129661000	-0.933751000
H	1.350965000	0.289193000	-1.141256000
S	-1.204732000	1.021790000	-0.124122000
H	-0.539719000	1.335778000	0.990337000
S	-1.111180000	-1.017496000	0.052720000
H	-2.262814000	-1.200181000	0.702014000

Conformer 4b

C	2.369656000	-0.264994000	-0.638393000
H	1.492699000	-0.645914000	-1.155427000
H	2.691229000	0.635403000	-1.154993000
H	3.164298000	-1.009016000	-0.713426000
N	1.993835000	0.078609000	0.730141000
H	1.683143000	-0.746138000	1.226506000
H	2.783248000	0.451872000	1.239490000
S	-1.379079000	-0.935818000	-0.047644000
H	-1.860891000	-1.026400000	1.193677000
S	-1.019743000	1.084585000	-0.094515000
H	0.252648000	0.999617000	0.358091000

Optimized conformers for the H_2S_2.methylammonium complex

Conformer 5a

C	-2.333170000	-0.534130000	-0.627999000
H	-1.558450000	-1.286217000	-0.719787000
H	-3.314781000	-0.991331000	-0.615262000
H	-2.257653000	0.182128000	-1.437072000
H	-1.170771000	0.620491000	0.654671000
H	-2.803382000	0.936350000	0.786794000
H	-2.186820000	-0.434261000	1.456693000
N	-2.118166000	0.192966000	0.656565000
S	1.598162000	-0.879778000	0.042911000
H	1.277993000	-1.045137000	1.329194000
S	0.844428000	1.013610000	-0.213468000
H	1.758613000	1.730692000	0.445716000

Conformer 5b

C	-2.477240000	0.381803000	0.539785000
H	-2.591447000	-0.274129000	1.393939000
H	-1.784568000	1.182687000	0.768645000
H	-3.436842000	0.785100000	0.240881000
H	-2.522871000	-1.181938000	-0.850584000
H	-1.767154000	0.171884000	-1.412642000
H	-0.984172000	-0.800853000	-0.325511000

N	-1.911125000	-0.410254000	-0.587757000
S	1.205423000	-1.007022000	0.081568000
H	1.476122000	-1.108419000	1.386049000
S	1.139418000	1.043608000	-0.062563000
H	2.334801000	1.221257000	-0.629272000

Conformer 5c

C	2.415346000	-0.260249000	-0.663889000
H	2.497398000	0.646083000	-1.251175000
H	3.377667000	-0.750965000	-0.586868000
H	1.678669000	-0.926292000	-1.096757000
H	1.017576000	0.570722000	0.638971000
H	1.847082000	-0.713937000	1.294119000
H	2.594120000	0.748847000	1.162531000
N	1.947521000	0.109712000	0.701948000
S	-1.310376000	-0.978768000	0.117436000
H	-2.142059000	-1.183563000	-0.906315000
S	-1.013608000	1.035064000	-0.178155000
H	-1.811449000	1.501886000	0.786686000

Optimized conformers for the H_2S_2.methylguanidinum complex

Conformer 6a

C	-1.949668000	-0.280666000	-0.129540000
H	-1.220597000	-1.513908000	-1.560636000
H	-0.126097000	-0.269980000	-1.076211000
N	-1.050779000	-0.685736000	-1.016736000
H	-3.008305000	-2.027418000	-0.114716000
N	-2.993983000	-1.061324000	0.158224000
N	-1.834227000	0.902113000	0.451417000
H	-3.792344000	-0.701004000	0.649384000
C	-0.851917000	1.907565000	0.079283000
H	0.114061000	1.694111000	0.529918000
H	-0.762172000	1.947741000	-1.002763000
H	-1.205346000	2.870138000	0.430506000
H	-2.428453000	1.086939000	1.242020000
S	2.194444000	0.212030000	-0.812367000
H	2.867160000	-0.808855000	-1.351001000
S	1.845321000	-0.591842000	1.045369000
H	2.888280000	-0.047533000	1.676677000

Conformer 6b

C	-1.540612000	0.305741000	0.135243000
H	0.028385000	-0.971340000	-0.149118000
H	-1.502267000	-1.527911000	-0.740535000
N	-0.961781000	-0.806201000	-0.298647000
H	0.208932000	1.318433000	0.421830000
N	-0.784723000	1.293468000	0.613670000
N	-2.861126000	0.420986000	0.111681000
H	-1.207822000	2.116501000	1.004219000
C	-3.756129000	-0.652419000	-0.284363000
H	-3.659943000	-0.876273000	-1.345062000
H	-3.563678000	-1.543503000	0.308299000
H	-4.772953000	-0.331293000	-0.093772000
H	-3.256107000	1.320584000	0.324920000
S	2.390796000	-1.061280000	0.343657000
H	2.110534000	-0.686222000	1.596094000
S	2.364480000	0.791010000	-0.547576000
H	3.564361000	1.227630000	-0.156382000

Conformer 6c

C	1.741519000	-0.520135000	0.145019000
H	3.493474000	-1.565401000	0.174177000
H	3.667736000	0.137461000	0.015289000
N	3.064461000	-0.661098000	0.093276000
H	1.383848000	-2.457304000	0.664596000
N	0.973086000	-1.570446000	0.433424000
N	1.192294000	0.658045000	-0.087374000
H	-0.020095000	-1.544466000	0.242012000
C	1.947318000	1.832548000	-0.483934000
H	2.593581000	2.181293000	0.320025000
H	2.534462000	1.625198000	-1.375644000
H	1.240136000	2.619529000	-0.718217000
H	0.201080000	0.766780000	0.106864000
S	-2.140696000	-0.757265000	-0.663702000
H	-3.371455000	-1.206570000	-0.405010000
S	-2.143239000	0.900392000	0.551922000
H	-1.921723000	0.293463000	1.722594000

Conformer 6d

C	-1.748185000	-0.548556000	-0.115897000
H	-3.449678000	-1.670311000	-0.212707000
H	-3.705950000	0.023765000	-0.076264000
N	-3.065180000	-0.747516000	-0.119143000
H	-1.280288000	-2.474987000	-0.582875000

N	-0.922862000	-1.568273000	-0.341046000
N	-1.263473000	0.658583000	0.115296000
H	0.069798000	-1.479106000	-0.158478000
C	-2.090861000	1.807753000	0.432097000
H	-2.710697000	2.098349000	-0.414673000
H	-2.712594000	1.603428000	1.300854000
H	-1.434371000	2.635519000	0.672764000
H	-0.269116000	0.804953000	-0.027426000
S	2.279152000	-0.780097000	0.571913000
H	3.251043000	-1.353413000	-0.142297000
S	2.052724000	0.911457000	-0.575188000
H	2.726708000	1.755301000	0.210559000

Optimized conformers for the H_2S_2.methanethiol complex

Conformer 7a

C	-1.874313000	0.203287000	1.139647000
H	-2.714934000	-0.238357000	1.666691000
H	-0.959591000	-0.266385000	1.488493000
H	-1.858873000	1.268931000	1.343409000
S	-2.139254000	-0.124217000	-0.613150000
H	-1.041718000	0.497924000	-1.041264000
S	1.592946000	0.996648000	-0.178597000
H	1.110683000	1.363947000	1.011208000
S	1.425792000	-1.034373000	0.049910000
H	2.638572000	-1.254701000	0.562975000

Conformer 7b

C	-1.808556000	-0.663227000	0.977228000
H	-1.308540000	-1.590621000	0.717938000
H	-1.171380000	-0.102871000	1.653905000
H	-2.758912000	-0.890442000	1.447486000
S	-2.053503000	0.222548000	-0.574678000
H	-2.748925000	1.239351000	-0.069382000
S	1.605261000	-0.951744000	-0.198847000
H	1.997138000	-0.831052000	-1.468743000
S	1.487497000	1.038193000	0.271742000
H	0.213885000	1.211029000	-0.116037000

Conformer 7c

C	1.932642000	-0.223273000	1.132201000
H	2.608415000	0.471429000	1.621920000

H	0.923623000	-0.044358000	1.490611000
H	2.240474000	-1.236947000	1.363411000
S	2.058196000	0.103036000	-0.636876000
H	1.174527000	-0.821392000	-1.012440000
S	-1.486779000	1.060976000	0.098837000
H	-0.220331000	1.179520000	-0.331825000
S	-1.589549000	-0.983523000	-0.003657000
H	-2.032454000	-1.096448000	-1.257753000

Optimized conformers for the H_2S_2.methanethiolate complex

Conformer 8a

C	-1.762728000	0.931465000	0.754394000
H	-1.387990000	1.835809000	0.283445000
H	-2.692834000	1.145144000	1.275913000
H	-1.019207000	0.570697000	1.461914000
S	-2.041518000	-0.367379000	-0.467663000
H	-0.752516000	-0.854850000	-0.328355000
S	1.709950000	0.814637000	-0.388298000
H	1.611891000	1.562905000	0.716885000
S	1.257632000	-1.062789000	0.359951000

Conformer 8b

C	1.790019000	0.625854000	0.988739000
H	1.843951000	1.699195000	0.829323000
H	0.817816000	0.373610000	1.411384000
H	2.578158000	0.319829000	1.671890000
S	1.926990000	-0.261655000	-0.580853000
H	0.667104000	-0.825318000	-0.439116000
S	-1.631062000	0.922877000	-0.223577000
H	-0.490417000	1.169481000	-0.885254000
S	-1.305724000	-1.066967000	0.271889000

Conformer 8c

C	1.912220000	0.957814000	0.726834000
H	1.022813000	0.825221000	1.348869000
H	2.780681000	0.950061000	1.387155000
H	1.846027000	1.945645000	0.268803000
S	2.023112000	-0.348872000	-0.527692000
S	-1.107944000	-1.011736000	0.394969000
H	0.146633000	-0.819982000	-0.015910000

S	-1.867423000	0.788206000	-0.231303000
H	-2.033393000	0.510607000	-1.525500000

Conformer 8d

C	-1.918918000	0.000420000	1.095538000
H	-0.938954000	0.000114000	1.579219000
H	-2.460036000	0.883094000	1.437374000
H	-2.460859000	-0.881539000	1.437914000
S	-1.737614000	-0.000223000	-0.710026000
S	1.403336000	1.043805000	0.033955000
H	0.135531000	1.020619000	-0.380400000
S	1.403184000	-1.043844000	0.034357000
H	0.135352000	-1.020601000	-0.379911000

Optimized conformers for the H_2S_2.dimethyl sulfide complex

Conformer 9a

C	1.535349000	-0.816476000	1.113168000
H	2.085624000	-1.616116000	1.601818000
H	1.299506000	-0.049647000	1.847505000
H	0.615694000	-1.220948000	0.697567000
S	2.583726000	-0.158969000	-0.183846000
C	1.473150000	1.106063000	-0.799627000
H	1.980383000	1.617686000	-1.613321000
H	0.555729000	0.661407000	-1.178324000
H	1.237906000	1.828567000	-0.021181000
S	-2.037567000	-0.842762000	-0.607321000
H	-2.319820000	-0.183644000	-1.733211000
S	-1.822416000	0.774885000	0.632576000
H	-3.085901000	0.854707000	1.055363000

Conformer 9b

C	3.105553000	-0.809442000	-0.182585000
H	3.111282000	-1.769991000	-0.689652000
H	3.804854000	-0.141754000	-0.680111000
H	3.408527000	-0.952687000	0.851844000
S	1.437382000	-0.158704000	-0.273437000
C	1.688895000	1.354113000	0.653582000
H	0.733735000	1.869886000	0.685568000
H	2.011087000	1.134165000	1.668567000
H	2.424937000	1.986289000	0.162282000
S	-2.067417000	-1.056837000	0.305112000
H	-0.759856000	-1.184948000	0.568578000
S	-1.986989000	0.907681000	-0.272265000

H	-1.628873000	0.716769000	-1.543614000

Conformer 9c

C	1.603848000	-0.458868000	1.392248000
H	1.621785000	-1.492974000	1.725264000
H	2.353342000	0.104768000	1.942622000
H	0.616300000	-0.042102000	1.576608000
S	1.970976000	-0.450715000	-0.363301000
C	1.823754000	1.313688000	-0.654046000
H	1.975839000	1.483821000	-1.716390000
H	0.833152000	1.661190000	-0.372250000
H	2.582265000	1.857638000	-0.096159000
S	-1.977405000	0.859312000	0.415398000
H	-2.212777000	1.561206000	-0.695433000
S	-1.739004000	-0.992162000	-0.437454000
H	-0.408593000	-0.925438000	-0.627756000

Optimized conformers for the H_2S_2.dimethyl disulfide complex

Conformer 10a

S	1.676723000	0.701516000	-0.769081000
S	2.194434000	-1.093634000	0.021563000
C	1.657066000	1.765226000	0.683357000
H	0.897616000	1.441606000	1.390653000
H	2.634113000	1.770779000	1.155764000
H	1.414956000	2.766765000	0.330451000
C	0.607425000	-1.738195000	0.575035000
H	-0.080213000	-1.823842000	-0.260985000
H	0.809404000	-2.726396000	0.985435000
H	0.179255000	-1.109284000	1.351022000
S	-1.952425000	1.054025000	0.263418000
H	-0.773519000	0.808271000	-0.330853000
S	-2.920663000	-0.654510000	-0.322994000
H	-2.637664000	-1.408425000	0.741664000

Conformer 10b

S	-2.015256000	-0.853590000	-0.077295000
S	-0.897021000	0.740782000	-0.650358000
C	-3.636877000	-0.113465000	0.171237000
H	-3.612080000	0.611813000	0.978920000
H	-3.980014000	0.353346000	-0.746345000
H	-4.308200000	-0.926140000	0.442437000

C	-0.432489000	1.459007000	0.932816000
H	0.127793000	0.737108000	1.520542000
H	0.200550000	2.314932000	0.707946000
H	-1.312757000	1.790454000	1.475787000
S	2.890062000	0.594261000	-0.121016000
H	3.253168000	0.396904000	-1.389906000
S	2.096765000	-1.254842000	0.258241000
H	0.854954000	-0.977445000	-0.166844000

Conformer 10c

S	-1.562769000	-1.039043000	-0.456006000
S	-2.364107000	0.745820000	0.080445000
C	-0.814101000	-1.602781000	1.082719000
H	-0.034268000	-0.917860000	1.404102000
H	-1.573316000	-1.702493000	1.852013000
H	-0.373815000	-2.576359000	0.871457000
C	-0.973349000	1.870243000	-0.125995000
H	-0.642711000	1.880963000	-1.160006000
H	-1.341394000	2.857837000	0.147613000
H	-0.151843000	1.600054000	0.531382000
S	2.155654000	-0.295848000	-1.055377000
H	0.831293000	-0.491529000	-0.956103000
S	2.473980000	0.488458000	0.813138000
H	2.766620000	-0.645578000	1.454014000

Conformer 10d

S	-1.214741000	-0.961689000	0.075811000
S	-1.234857000	0.825391000	-0.886671000
C	-2.942637000	-1.146513000	0.546532000
H	-3.241646000	-0.368560000	1.242522000
H	-3.575404000	-1.128691000	-0.334949000
H	-3.025082000	-2.114821000	1.036887000
C	-1.082864000	2.001851000	0.468191000
H	-0.160558000	1.823110000	1.011370000
H	-1.055542000	2.989984000	0.011879000
H	-1.942079000	1.938941000	1.129467000
S	2.257261000	0.182208000	1.042071000
H	1.372761000	-0.695136000	1.524140000
S	2.348200000	-0.527862000	-0.878437000
H	1.286758000	0.134378000	-1.354053000

Optimized conformers for the H_2S_2.methanol complex

Conformer 11a

C	2.474815000	0.201492000	-0.522942000
H	3.328659000	0.851238000	-0.360822000
H	2.794091000	-0.644302000	-1.133202000
H	1.711871000	0.761644000	-1.065918000
O	2.018924000	-0.208311000	0.751244000
H	1.228345000	-0.736685000	0.614793000
S	-1.127822000	1.026039000	0.097427000
H	-2.321286000	1.272969000	-0.446760000
S	-1.128168000	-1.006054000	-0.189141000
H	-1.646121000	-1.367085000	0.987035000

Conformer 11b

C	2.384071000	-0.614514000	-0.422337000
H	1.465635000	-1.188328000	-0.481840000
H	2.599809000	-0.191170000	-1.402596000
H	3.196159000	-1.277746000	-0.127902000
O	2.161636000	0.398825000	0.549315000
H	2.959628000	0.922279000	0.632163000
S	-1.062288000	1.066387000	-0.177454000
H	0.232910000	1.028699000	0.163977000
S	-1.455170000	-0.933379000	0.052876000
H	-1.772322000	-0.925382000	1.348938000

Conformer 11c

C	-3.133842000	0.082719000	0.035923000
H	-3.726763000	-0.819533000	0.140281000
H	-3.309568000	0.715869000	0.905598000
H	-3.459508000	0.609965000	-0.860552000
O	-1.780836000	-0.321154000	-0.055895000
H	-1.229397000	0.461112000	-0.149027000
S	1.475006000	-0.983862000	0.012528000
H	0.177714000	-1.297772000	0.096192000
S	1.232682000	1.051626000	-0.082858000
H	1.274246000	1.319061000	1.224415000

Conformer 11d

C	2.460290000	0.017168000	-0.526750000
H	3.166224000	0.840065000	-0.490456000
H	2.992716000	-0.888493000	-0.815650000
H	1.701939000	0.239375000	-1.279461000

O	1.893810000	-0.097928000	0.767557000
H	1.233395000	-0.795817000	0.725865000
S	-1.203348000	-0.980465000	-0.146728000
H	-1.733783000	-1.235668000	1.051388000
S	-1.132338000	1.066830000	-0.020499000
H	0.098262000	1.139111000	0.503997000

Optimized conformers for the H_2S_2.acetic acid complex

Conformer 12a

C	1.640707000	-0.234871000	1.400316000
H	1.875737000	0.685212000	1.920185000
H	2.300281000	-1.029770000	1.742514000
H	0.618134000	-0.539078000	1.604481000
C	1.839847000	-0.042453000	-0.065591000
O	2.383402000	0.888760000	-0.599678000
O	1.351506000	-1.094545000	-0.772819000
H	1.548836000	-0.898134000	-1.698378000
S	-2.034625000	-0.813653000	0.014983000
H	-0.867521000	-1.377479000	-0.310646000
S	-1.381380000	1.128945000	0.044673000
H	-1.581977000	1.424805000	-1.241027000

Conformer 12b

C	1.536971000	1.190217000	0.580308000
H	0.480500000	1.283146000	0.357088000
H	2.080557000	2.068318000	0.246396000
H	1.674277000	1.101834000	1.656237000
C	2.084272000	-0.036364000	-0.068002000
O	1.434444000	-0.961278000	-0.498934000
O	3.428586000	-0.026921000	-0.111343000
H	3.690588000	-0.862260000	-0.520447000
S	-1.854700000	-1.015775000	0.386937000
H	-0.570299000	-1.084829000	0.009452000
S	-2.233119000	0.883828000	-0.286934000
H	-2.582225000	0.587412000	-1.540397000

Conformer 12c

C	-3.424549000	-0.100291000	-0.030234000
H	-3.797622000	-1.103163000	0.132990000
H	-3.749782000	0.270206000	-0.998713000
H	-3.815171000	0.575226000	0.726133000
C	-1.931675000	-0.099531000	0.026013000
O	-1.245815000	-1.078727000	0.227365000

O	-1.428788000	1.122261000	-0.173185000
H	-0.454723000	1.064974000	-0.117913000
S	2.058009000	-1.013279000	-0.113927000
H	0.755936000	-1.297155000	0.045142000
S	1.856656000	1.024495000	0.017810000
H	1.960896000	1.161113000	1.342120000

Optimized conformers for the H_2S_2.acetate complex

Conformer 13a

C	3.281686000	-0.171639000	-0.305167000
H	3.346212000	-0.352861000	-1.377080000
H	3.754899000	-0.987671000	0.234568000
H	3.806688000	0.760711000	-0.103002000
C	1.808300000	-0.024236000	0.092948000
O	1.340078000	-0.829799000	0.918139000
O	1.203646000	0.933200000	-0.483435000
S	-2.058477000	-0.897756000	-0.397766000
H	-1.791925000	-1.577851000	0.718467000
S	-1.668150000	0.991701000	0.295991000
H	-0.379545000	1.002597000	-0.048874000

Conformer 13b

C	-3.303734000	-0.908411000	-0.005631000
H	-3.252425000	-1.530386000	-0.896187000
H	-4.240718000	-0.363008000	0.015453000
H	-3.234446000	-1.567704000	0.856399000
C	-2.141282000	0.057536000	0.002397000
O	-2.296734000	1.264380000	0.026006000
O	-0.995528000	-0.581324000	-0.019426000
H	-0.175616000	0.059636000	-0.015527000
S	1.518099000	0.985618000	-0.001346000
S	2.677990000	-0.731133000	-0.074801000
H	2.773969000	-1.029500000	1.224977000

Conformer 13c

C	3.240258000	-0.007044000	0.029072000
H	3.568790000	-0.183952000	1.051467000
H	3.665163000	0.921245000	-0.341296000
H	3.593296000	-0.841614000	-0.573924000
C	1.714947000	0.027634000	-0.010743000
O	1.169896000	1.060677000	-0.466110000
O	1.142140000	-1.010483000	0.426650000

S	-1.854189000	0.997655000	0.241096000
H	-0.550618000	1.205650000	-0.136861000
S	-1.776291000	-1.029486000	-0.235634000
H	-0.416463000	-1.117132000	0.118928000

Conformer 13d

C	-1.353510000	-0.926049000	0.903847000
H	-0.482769000	-1.376847000	0.429325000
H	-2.050269000	-1.685407000	1.241443000
H	-0.970802000	-0.350620000	1.743580000
C	-2.046741000	-0.010447000	-0.067132000
O	-3.216949000	-0.138060000	-0.376556000
O	-1.302852000	0.957332000	-0.577809000
H	-0.354299000	0.939944000	-0.214806000
S	2.095953000	-0.854547000	-0.354706000
H	2.051953000	-0.598938000	-1.666207000
S	1.551929000	0.988088000	0.422287000

Optimized conformers for the H_2S_2.toluene complex

Conformer 14a

C	-1.104454000	1.126354000	-0.038099000
C	-0.907028000	0.526200000	1.205691000
C	-1.367619000	-0.760428000	1.461564000
C	-2.043437000	-1.468192000	0.473801000
C	-2.263809000	-0.877453000	-0.765656000
C	-1.797175000	0.408820000	-1.014337000
H	-0.376244000	1.071611000	1.975704000
H	-1.197724000	-1.210034000	2.430854000
H	-2.398705000	-2.470790000	0.669428000
H	-2.794847000	-1.416621000	-1.538661000
H	-1.961050000	0.860994000	-1.985079000
C	-0.531925000	2.476132000	-0.338202000
H	-0.470880000	3.087520000	0.559621000
H	0.478870000	2.373601000	-0.735208000
H	-1.130328000	3.004700000	-1.077354000
S	2.537706000	0.246390000	0.442008000
H	2.531336000	-0.546712000	1.515876000
S	1.651684000	-1.037063000	-0.884686000
H	0.382006000	-0.692094000	-0.640918000

Optimized conformers for the H_2S_2.3-methylindole complex

Conformer 15a

C	-1.120619000	0.703007000	-0.205638000
C	-1.400367000	-0.027309000	0.977588000
C	-2.450415000	-0.938878000	1.061013000
C	-3.225189000	-1.118000000	-0.071478000
C	-2.962554000	-0.411358000	-1.258207000
C	-1.921360000	0.494695000	-1.337177000
C	0.027326000	1.510945000	0.048594000
C	0.394391000	1.256463000	1.349330000
H	-2.651088000	-1.489618000	1.970972000
H	-4.047724000	-1.819931000	-0.043574000
H	-3.588798000	-0.582966000	-2.123265000
H	-1.723974000	1.031900000	-2.256321000
H	1.217453000	1.658702000	1.917039000
H	-0.397443000	-0.020862000	2.839436000
N	-0.461382000	0.338585000	1.903967000
C	0.719357000	2.396365000	-0.924605000
H	1.098406000	1.820593000	-1.770550000
H	0.044970000	3.156290000	-1.318882000
H	1.565181000	2.899205000	-0.460477000
S	1.671800000	-1.512376000	-0.648436000
H	0.739825000	-0.571001000	-0.436148000
S	3.285931000	-0.416630000	-0.022994000
H	3.285761000	-0.783892000	1.260367000

Conformer 15b

C	1.411689000	0.149771000	-0.028705000
C	0.477711000	0.552505000	0.958502000
C	-0.047167000	1.842603000	1.008550000
C	0.371682000	2.734851000	0.036414000
C	1.295359000	2.356969000	-0.954320000
C	1.822425000	1.079542000	-0.993037000
C	1.705812000	-1.226828000	0.195164000
C	0.955896000	-1.606881000	1.284922000
H	-0.749905000	2.135906000	1.778077000
H	-0.014504000	3.745504000	0.043118000
H	1.598251000	3.083463000	-1.696220000
H	2.532940000	0.799383000	-1.760566000
H	0.889134000	-2.567383000	1.770074000
H	-0.464659000	-0.578399000	2.471549000
N	0.231424000	-0.536216000	1.748169000
C	2.629173000	-2.076799000	-0.603597000
H	2.330240000	-2.105048000	-1.651636000

H	3.649046000	-1.694444000	-0.565669000
H	2.640271000	-3.099032000	-0.230688000
S	-1.759373000	-1.063026000	-1.239785000
H	-0.662032000	-1.256957000	-0.496571000
S	-2.906922000	-0.104258000	0.159821000
H	-2.443518000	1.132662000	-0.042577000

Conformer 15c

C	1.381654000	0.269602000	0.025547000
C	0.430472000	0.306724000	1.077632000
C	-0.323779000	1.441715000	1.364830000
C	-0.120924000	2.555678000	0.565884000
C	0.817737000	2.543953000	-0.482529000
C	1.573977000	1.417028000	-0.753947000
C	1.909356000	-1.050801000	-0.030591000
C	1.273009000	-1.759125000	0.959761000
H	-1.055210000	1.447453000	2.162155000
H	-0.696232000	3.452747000	0.752333000
H	0.946476000	3.433966000	-1.083881000
H	2.288179000	1.415924000	-1.568027000
H	1.382556000	-2.794154000	1.240900000
H	-0.229714000	-1.234097000	2.358627000
N	0.394267000	-0.941947000	1.628073000
C	2.919907000	-1.557832000	-0.996842000
H	2.561085000	-1.462946000	-2.021869000
H	3.853596000	-1.000745000	-0.922411000
H	3.141258000	-2.607900000	-0.816305000
S	-1.659226000	-0.278815000	-1.481005000
H	-1.129101000	0.825715000	-0.938500000
S	-2.662888000	-0.942260000	0.175310000
H	-3.837393000	-0.346786000	-0.046896000

Conformer 15d

C	0.649086000	0.808733000	0.476853000
C	1.318163000	0.451979000	-0.720829000
C	2.230221000	-0.598397000	-0.782498000
C	2.464761000	-1.304432000	0.385115000
C	1.804336000	-0.976347000	1.583458000
C	0.903281000	0.073403000	1.641434000
C	-0.227478000	1.890963000	0.175073000
C	-0.074649000	2.142339000	-1.168808000
H	2.727846000	-0.862610000	-1.706755000
H	3.164770000	-2.129145000	0.374583000
H	2.008328000	-1.556214000	2.473659000
H	0.394356000	0.313848000	2.566350000

H	-0.556846000	2.883001000	-1.786506000
H	1.118792000	1.245287000	-2.669071000
N	0.855533000	1.284524000	-1.700867000
C	-1.118921000	2.596747000	1.134208000
H	-1.795400000	1.896506000	1.626491000
H	-0.542607000	3.093894000	1.914376000
H	-1.720670000	3.350834000	0.630054000
S	-1.041683000	-2.038229000	-0.668022000
H	-0.095116000	-1.868821000	0.264393000
S	-2.480763000	-0.848657000	0.177953000
H	-2.025859000	0.322007000	-0.284442000

Conformer 15e

C	1.063867000	0.510565000	-0.302076000
C	0.645663000	0.658303000	1.044461000
C	-0.185556000	1.698166000	1.456312000
C	-0.567816000	2.622573000	0.497440000
C	-0.137055000	2.514320000	-0.837459000
C	0.668481000	1.467712000	-1.245777000
C	1.855452000	-0.672180000	-0.377873000
C	1.906746000	-1.180712000	0.900210000
H	-0.516003000	1.786387000	2.483290000
H	-1.208119000	3.446414000	0.783537000
H	-0.452433000	3.259735000	-1.555101000
H	0.979122000	1.381228000	-2.279309000
H	2.411013000	-2.060300000	1.267416000
H	1.004691000	-0.579890000	2.716602000
N	1.193346000	-0.375289000	1.751565000
C	2.501678000	-1.226625000	-1.597934000
H	1.762091000	-1.440055000	-2.369684000
H	3.219172000	-0.521951000	-2.018175000
H	3.031077000	-2.150945000	-1.375069000
S	-1.605241000	-1.874532000	0.439494000
H	-0.332330000	-1.877470000	0.020388000
S	-2.322941000	-0.474608000	-0.873277000
H	-1.909540000	0.617362000	-0.218128000

Optimized conformers for the H_2S_2.4-methylphenol complex

Conformer 16a

C	-1.381359000	-0.100274000	1.244923000
C	-2.104043000	-0.417445000	0.100648000
C	-1.876975000	0.283651000	-1.075926000
C	-0.925775000	1.294403000	-1.099011000

C	-0.186114000	1.629285000	0.033631000
C	-0.432042000	0.913156000	1.203314000
H	-1.546393000	-0.653420000	2.162267000
H	-2.440519000	0.022184000	-1.960832000
H	-0.752553000	1.831877000	-2.023815000
H	0.135521000	1.141899000	2.096985000
O	-3.032726000	-1.416442000	0.068865000
H	-3.082985000	-1.819714000	0.938718000
C	0.814176000	2.744467000	0.010894000
H	1.637234000	2.544431000	0.694759000
H	1.224534000	2.886852000	-0.987811000
H	0.354924000	3.686067000	0.312546000
S	2.720747000	-0.496953000	0.162631000
H	2.536259000	0.457783000	-0.752103000
S	1.093001000	-1.649256000	-0.314400000
H	1.728612000	-2.510534000	-1.114160000

Conformer 16b

C	1.297986000	-0.336916000	1.289914000
C	2.116204000	-0.583851000	0.194850000
C	2.048021000	0.245063000	-0.918813000
C	1.146392000	1.301984000	-0.938170000
C	0.299731000	1.554860000	0.138219000
C	0.403321000	0.723214000	1.253338000
H	1.376098000	-0.977439000	2.157884000
H	2.695157000	0.065289000	-1.769521000
H	1.093939000	1.934842000	-1.815837000
H	-0.233583000	0.906759000	2.109619000
O	2.971884000	-1.643195000	0.276714000
H	3.478548000	-1.695311000	-0.537031000
C	-0.729082000	2.640274000	0.078796000
H	-1.678842000	2.240658000	-0.280415000
H	-0.905401000	3.072636000	1.061763000
H	-0.425109000	3.437146000	-0.596989000
S	-2.664730000	-0.732667000	0.520355000
H	-2.000984000	-1.528412000	1.362272000
S	-1.375619000	-0.875469000	-1.068967000
H	-2.024749000	-1.848194000	-1.716464000

Conformer 16c

C	-1.286160000	-0.303854000	1.297385000
C	-2.090275000	-0.655524000	0.218957000
C	-2.078857000	0.123436000	-0.932404000
C	-1.251047000	1.239490000	-1.002144000
C	-0.423743000	1.600383000	0.060090000

C	-0.468684000	0.813261000	1.212141000
H	-1.313653000	-0.913052000	2.190463000
H	-2.710873000	-0.138724000	-1.772747000
H	-1.242046000	1.833144000	-1.908138000
H	0.158093000	1.074615000	2.055329000
O	-2.869166000	-1.764301000	0.355321000
H	-3.365724000	-1.899691000	-0.455234000
C	0.525630000	2.752848000	-0.046147000
H	0.565624000	3.316699000	0.883957000
H	1.534018000	2.393921000	-0.255986000
H	0.236096000	3.431367000	-0.845639000
S	1.588139000	-1.160698000	-1.047831000
H	0.552782000	-0.328559000	-0.878149000
S	2.710597000	-0.512107000	0.536606000
H	2.198040000	-1.310671000	1.475903000

Conformer 16d

C	0.824130000	1.222245000	-1.179611000
C	0.132151000	1.594914000	-0.033931000
C	0.449013000	1.008028000	1.185993000
C	1.457752000	0.052577000	1.250067000
C	2.166174000	-0.336752000	0.113965000
C	1.829160000	0.268932000	-1.096538000
H	0.559024000	1.676597000	-2.124351000
H	-0.098454000	1.283444000	2.079154000
H	1.688060000	-0.404890000	2.204625000
H	2.354842000	-0.020049000	-1.998508000
O	-0.853503000	2.525765000	-0.169513000
H	-1.298288000	2.626732000	0.676132000
C	3.266319000	-1.350706000	0.194981000
H	3.328249000	-1.937115000	-0.719540000
H	4.230942000	-0.864978000	0.341630000
H	3.110577000	-2.034550000	1.026798000
S	-1.334609000	-1.747431000	-0.418238000
H	-0.240701000	-1.146688000	0.067332000
S	-2.720204000	-0.415079000	0.287824000
H	-2.677417000	0.460113000	-0.720095000

Conformer 16e

C	0.371504000	0.884049000	1.212509000
C	0.175631000	1.568087000	0.019319000
C	0.971126000	1.283924000	-1.082883000
C	1.948021000	0.299462000	-0.992817000
C	2.147413000	-0.420080000	0.183197000
C	1.344480000	-0.103254000	1.281089000

H	-0.255081000	1.113950000	2.062448000
H	0.813160000	1.810344000	-2.016789000
H	2.555018000	0.078453000	-1.862201000
H	1.476501000	-0.645919000	2.209436000
O	-0.839537000	2.481252000	-0.018348000
H	-0.864558000	2.882198000	-0.891097000
C	3.205911000	-1.475927000	0.282984000
H	4.100749000	-1.083457000	0.765655000
H	2.860174000	-2.324110000	0.870882000
H	3.492300000	-1.839878000	-0.701314000
S	-1.441468000	-1.345651000	-0.918624000
H	-0.272566000	-1.201785000	-0.279792000
S	-2.661062000	-0.625259000	0.561135000
H	-2.533441000	0.677183000	0.288973000

Optimized conformers for the H_2S_2.4-methylimidazole complex

Conformer 17a

C	-2.242608000	-1.006111000	-0.291223000
C	-1.236232000	0.867069000	-0.014011000
C	-1.084273000	0.166559000	1.161947000
N	-1.734936000	-1.019145000	0.967282000
H	-1.797323000	-1.776372000	1.624914000
H	-2.806334000	-1.827807000	-0.698085000
H	-0.576351000	0.403592000	2.079417000
N	-1.962460000	0.125428000	-0.907407000
C	-0.698741000	2.203927000	-0.369756000
H	-0.169856000	2.647299000	0.471037000
H	-0.008464000	2.119455000	-1.208750000
H	-1.501330000	2.874840000	-0.669693000
S	2.466091000	0.178534000	0.529123000
H	2.654608000	1.252559000	-0.240845000
S	1.249003000	-0.881675000	-0.738632000
H	2.216448000	-1.575969000	-1.346714000

Conformer 17b

C	-2.121656000	-1.171758000	-0.259656000
C	-1.321434000	0.817584000	-0.107055000
C	-1.252826000	0.270957000	1.154606000
N	-1.765559000	-0.990706000	1.037027000
H	-1.858866000	-1.665379000	1.776393000
H	-2.553735000	-2.088448000	-0.621904000
H	-0.890028000	0.662737000	2.087719000
N	-1.865529000	-0.094798000	-0.977918000

C	-0.865851000	2.153867000	-0.565163000
H	-0.514174000	2.752102000	0.271831000
H	-0.047857000	2.053900000	-1.277976000
H	-1.675751000	2.684162000	-1.061617000
S	2.337066000	0.391199000	0.594313000
H	2.091361000	-0.351044000	1.675999000
S	1.653552000	-0.915630000	-0.827092000
H	0.387390000	-0.482521000	-0.876116000

Conformer 17c

C	-0.654076000	-1.371245000	-0.722238000
C	-2.011233000	0.151533000	-0.043003000
C	-1.628735000	-0.557797000	1.072145000
N	-0.770711000	-1.520634000	0.618947000
H	-0.284483000	-2.196916000	1.181932000
H	-0.025261000	-2.002585000	-1.325051000
H	-1.881595000	-0.455731000	2.112222000
N	-1.393241000	-0.364603000	-1.154728000
C	-2.927648000	1.316592000	-0.134936000
H	-3.310561000	1.588620000	0.845955000
H	-2.412311000	2.179177000	-0.553749000
H	-3.770883000	1.090862000	-0.784519000
S	1.461290000	1.276294000	0.210110000
H	0.417054000	0.815747000	-0.492366000
S	2.690941000	-0.344339000	-0.029791000
H	3.310168000	0.031696000	-1.150887000

Conformer 17d

C	-1.504135000	-1.499767000	0.571704000
C	-1.730249000	0.494292000	-0.191027000
C	-1.060552000	-0.220700000	-1.160210000
N	-0.931242000	-1.484535000	-0.657853000
H	-0.455226000	-2.251214000	-1.101122000
H	-1.528653000	-2.379910000	1.190460000
H	-0.673497000	0.057725000	-2.123601000
N	-2.000237000	-0.317814000	0.882279000
C	-2.135097000	1.923184000	-0.207345000
H	-1.821057000	2.405491000	-1.130282000
H	-3.215655000	2.015990000	-0.118967000
H	-1.689498000	2.457440000	0.630067000
S	1.613388000	0.257129000	1.147886000
H	0.350108000	0.420686000	0.730250000
S	2.472783000	0.018590000	-0.695951000
H	2.755288000	1.296676000	-0.957476000

Conformer 17e

C	0.851608000	-1.199158000	-0.116353000
C	2.159654000	0.502730000	0.067137000
C	2.968171000	-0.605367000	-0.026876000
N	2.119887000	-1.672871000	-0.142459000
H	2.387604000	-2.637521000	-0.230812000
H	-0.020081000	-1.826357000	-0.186844000
H	4.037462000	-0.717712000	-0.021044000
N	0.845981000	0.115204000	0.009882000
C	2.543502000	1.930284000	0.207641000
H	3.624685000	2.040530000	0.244375000
H	2.167754000	2.513011000	-0.631155000
H	2.123739000	2.351914000	1.118738000
S	-2.296207000	1.130047000	-0.249324000
H	-0.962772000	0.928459000	-0.149548000
S	-2.849076000	-0.805057000	0.156174000
H	-2.932553000	-0.719432000	1.485435000

Conformer 17f

C	1.273445000	-1.000622000	1.147453000
C	1.414340000	0.733422000	-0.116788000
C	1.960647000	-0.312985000	-0.822903000
N	1.867910000	-1.400783000	-0.001729000
H	2.159899000	-2.336806000	-0.221670000
H	1.078985000	-1.668571000	1.968528000
H	2.390188000	-0.369219000	-1.807012000
N	0.997805000	0.290553000	1.112867000
C	1.240914000	2.147520000	-0.534329000
H	1.677805000	2.318466000	-1.515549000
H	0.183424000	2.403976000	-0.580096000
H	1.717045000	2.818358000	0.177890000
S	-2.180477000	0.647301000	0.484242000
H	-0.993488000	0.707208000	1.118976000
S	-1.662347000	-0.872908000	-0.789978000
H	-2.124751000	-1.896093000	-0.067855000

Optimized conformers for the H_2S_2.4-methylimidazolium complex

Conformer 18a

C	-0.909820000	-1.286605000	-0.248217000
C	-2.092399000	0.564409000	0.109807000
C	-2.958961000	-0.491323000	0.003747000
N	-2.201784000	-1.609748000	-0.215584000

H	-2.556912000	-2.546582000	-0.337245000
H	-0.078303000	-1.950551000	-0.402956000
H	-4.031177000	-0.524149000	0.066509000
C	-2.326206000	2.008306000	0.340096000
H	-1.946491000	2.598193000	-0.491266000
H	-3.390317000	2.199382000	0.436029000
H	-1.835633000	2.339237000	1.252763000
H	0.042675000	0.549508000	-0.046969000
N	-0.839465000	0.028039000	-0.049606000
S	2.754639000	-0.818142000	0.376217000
H	2.061474000	-0.701512000	1.512786000
S	2.230394000	0.976959000	-0.477516000
H	2.987211000	1.798647000	0.254877000

Conformer 18b

C	-1.936553000	-1.404557000	-0.194259000
C	-1.558367000	0.754022000	0.178959000
C	-2.891919000	0.586848000	-0.086495000
N	-3.090075000	-0.747964000	-0.311132000
H	-3.973113000	-1.183166000	-0.533178000
H	-1.787668000	-2.461818000	-0.316522000
H	-3.691390000	1.303454000	-0.130192000
C	-0.763303000	1.964386000	0.486934000
H	-0.017410000	2.141344000	-0.285014000
H	-1.415377000	2.830733000	0.539273000
H	-0.254047000	1.861178000	1.442752000
H	-0.013718000	-0.721392000	0.253811000
N	-1.007027000	-0.500393000	0.102338000
S	2.204723000	-1.104800000	0.350472000
H	2.586120000	-0.834377000	1.602203000
S	2.568796000	0.727065000	-0.501455000
H	3.770871000	0.442113000	-1.006676000

Conformer 18c

C	-1.861924000	-1.440715000	0.054908000
C	-1.502368000	0.741320000	-0.181435000
C	-2.797873000	0.556591000	0.224216000
N	-2.985380000	-0.791866000	0.359513000
H	-3.842304000	-1.241357000	0.646048000
H	-1.714100000	-2.504907000	0.072941000
H	-3.577829000	1.269209000	0.420214000
C	-0.730239000	1.965709000	-0.491742000
H	-0.435416000	1.980450000	-1.539096000
H	-1.335132000	2.845166000	-0.294352000
H	0.166722000	2.014008000	0.122808000

H	0.009136000	-0.707064000	-0.547239000
N	-0.962606000	-0.517115000	-0.273086000
S	2.232490000	-0.441845000	-0.896898000
H	2.805096000	-1.644210000	-0.787451000
S	2.357411000	0.150781000	1.066324000
H	3.475737000	0.871169000	0.954645000

Conformer 18d

C	-0.815004000	0.947184000	-0.275742000
C	-2.742988000	-0.126078000	0.045267000
C	-1.712786000	-1.022132000	0.156685000
N	-0.549246000	-0.333967000	-0.044668000
H	0.399522000	-0.724831000	-0.031760000
H	-0.091874000	1.719118000	-0.467130000
H	-1.729555000	-2.077262000	0.359422000
C	-4.209509000	-0.291139000	0.164310000
H	-4.708837000	-0.011353000	-0.760799000
H	-4.445326000	-1.328978000	0.376804000
H	-4.605551000	0.320102000	0.972383000
H	-2.629319000	1.953394000	-0.361514000
N	-2.142216000	1.079972000	-0.222454000
S	2.637047000	-1.043092000	-0.251791000
H	3.144910000	-1.588707000	0.856744000
S	2.770124000	0.932940000	0.300022000
H	3.873266000	1.231904000	-0.389121000

Optimized conformers for the H_2S_2.4-methylphenolate complex

Conformer 19a

C	0.889521000	1.244717000	-1.117718000
C	-0.006752000	1.452125000	-0.030401000
C	0.375684000	0.797765000	1.176846000
C	1.475712000	-0.049255000	1.250012000
C	2.302733000	-0.279635000	0.148799000
C	1.988693000	0.404457000	-1.029773000
H	0.645347000	1.727388000	-2.057470000
H	-0.259443000	0.940126000	2.043424000
H	1.694229000	-0.551157000	2.189211000
H	2.615220000	0.259634000	-1.906285000
O	-1.102607000	2.116922000	-0.143277000
C	3.508558000	-1.166865000	0.242705000
H	3.691585000	-1.688027000	-0.697842000
H	4.413953000	-0.602550000	0.481644000
H	3.381743000	-1.920778000	1.020210000
S	-2.741217000	-0.333823000	0.470834000

H	-2.193609000	0.842884000	0.162548000
S	-1.508912000	-1.484265000	-0.713464000
H	-0.371001000	-1.273355000	-0.049966000

Conformer 19b

C	1.820977000	1.619489000	0.292708000
C	0.552477000	1.057237000	0.126524000
C	0.456547000	-0.315870000	-0.130122000
C	1.610195000	-1.083080000	-0.223945000
C	2.882534000	-0.533508000	-0.066008000
C	2.961966000	0.832483000	0.198127000
H	1.891208000	2.679789000	0.498914000
H	-0.524743000	-0.763169000	-0.231113000
H	1.512342000	-2.146191000	-0.417389000
H	3.935573000	1.291800000	0.334492000
O	-0.517541000	1.853086000	0.239048000
C	4.115640000	-1.375628000	-0.208569000
H	4.392396000	-1.503043000	-1.256614000
H	4.963986000	-0.920502000	0.301667000
H	3.965454000	-2.369830000	0.211413000
H	-1.354660000	1.357375000	-0.031448000
S	-3.079006000	0.471114000	-0.649552000
S	-3.040214000	-1.275258000	0.464425000
H	-3.135726000	-0.791344000	1.707446000

Conformer 19c

C	0.988539000	1.192979000	0.581945000
C	0.300644000	-0.003430000	0.914850000
C	0.995183000	-1.196988000	0.585449000
C	2.254633000	-1.189153000	0.001119000
C	2.914210000	0.002006000	-0.305444000
C	2.247989000	1.190370000	-0.002429000
H	0.492521000	2.132396000	0.800503000
H	0.504328000	-2.138446000	0.806895000
H	2.736808000	-2.135261000	-0.229401000
H	2.724878000	2.138458000	-0.235772000
O	-0.874402000	-0.006042000	1.460426000
C	4.294446000	0.004998000	-0.893041000
H	4.456350000	0.885468000	-1.515585000
H	5.066621000	0.007740000	-0.119707000
H	4.460932000	-0.875798000	-1.513918000
S	-2.922060000	1.050129000	-0.488317000
H	-1.975232000	1.008285000	0.450471000
S	-2.919981000	-1.047728000	-0.502812000
H	-1.973203000	-1.017609000	0.436475000

FF for H_2S_2 and parameters for its interactions with amino acid side chains

Copy the following lines into a "name.str" file and stream it after reading the main FF topology and parameter files

```
* Topology and parameter for hydrogen persulfide (H2S2)
* January 2019
*

set nat ?NATC
set app
if "@NAT" ne "?NATC" if @nat ne 0 set app append

read rtf card @app
* Topology for water and ions
*
31  1

MASS  1  HPER    1.00800 H ! H of H2S2
MASS  2  SPER   32.06000 S ! S of H2S2

DEFA FIRS NONE LAST NONE
AUTOGENERATE ANGLES DIHEDRALS

RESI H2S2        0.000 ! Hydrogen persulfide
!   HP1
!     \
!     SP1--SP2
!             \
!            HP2
GROUP
ATOM HP1   HPER   0.155
ATOM SP1   SPER   -0.155
ATOM SP2   SPER   -0.155
ATOM HP2   HPER   0.155

BOND  HP1 SP1  SP1 SP2  SP2 HP2
DONOR HP1 SP1
DONOR HP2 SP2
ACCEPTOR SP1
ACCEPTOR SP2
IC HP1  SP1  SP2  HP2   1.342  98.1  90.7  98.1  1.342
PATCH FIRST NONE LAST NONE

end

read para card flex @app
* Parameters for water and ions
*

ATOMS
MASS  1  HPER    1.00800 H ! H of H2S2
MASS  2  SPER   32.06000 S  ! S of H2S2

BONDS
!atom    type     Kb         b0
```

```
!=============================================
HPER  SPER   271.0     1.342
SPER  SPER   189.5     2.059


ANGLES
!atom    types              Ktheta    Theta
!=============================================
HPER  SPER  SPER       55.5    98.1


DIHEDRALS
!atom    types                    Kchi    n     delta
!=============================================
HPER  SPER  SPER  HPER   3.17     2     0.0

!!!!Warning
! The following values are for gas-phase calculations only
! Reset to defaults values when running MD simulations

NONBONDED nbxmod  5 atom cdiel fshift vatom vdistance vfswitch -
cutnb 2000.0 ctofnb 1950.0 ctonnb 1900.0 eps 1.0 e14fac 1.0 wmin 1.5

HPER       0.0      -0.1140      0.8980
SPER       0.0      -0.4115      2.0590

NBFIX

SPER  OB      -1.35820     3.47886   ! H2S2-acetic, acetamide and NMA
SPER  OH1     -0.67513     3.50662   ! H2S2-acetic, MeOH and mephenol
SPER   O        -1.35820     3.47886   ! H2S2-acetamide
SPER   NH2    -1.34643     3.34590   ! H2S2-acetamide, Methylamine, Methylammonium, and Methylimidazolium
SPER   S         -1.15820     3.82945   ! H2S2-DMS, CH3SH
SPER   NC2     -0.97580     3.64273   ! H2S2-methylguandinium
SPER  OC        -2.76320     3.23160   ! H2S2-acetate
HPER  OC         -0.0          0.0          ! H2S2-acetate
SPER  SS         -5.98200     3.41132   ! H2S2-methanethiolate
HPER  SS          -0.0           0.0          ! H2S2-methanethiolate

END
return
```