

Table S1: Harmonic vibrational frequencies in cm^{-1} and percentage errors Δ (see text for details).

Mol	HCTH-93	$\Delta_{\text{HCTH-93}}$	1/4	$\Delta_{1/4}$	MP2	Δ_{MP2}	Expt.	Ref.
H ₂ S								
<i>A</i> ₁	2670	-2.1	2693	-1.2	2780	1.9	2727	[44]
	1181	-0.2	1174	-0.8	1211	2.4	1183	[44]
<i>B</i> ₂	2688	-1.9	2711	-1.0	2799	2.2	2739	[44]
OCS								
Σ^+	2098	1.7	2123	3.0	2100	1.8	2062	[44]
	874	1.7	892	3.8	890	3.6	859	[44]
Π	513	-1.3	519	-0.2	523	0.6	520	[44]
CS ₂								
Σ_u	1565	2.1	1594	4.0	1625	6.0	1533	[44]
Σ_g	667	1.4	681	3.5	676	2.7	658	[44]
Π_u	394	-0.8	400	0.8	402	1.3	397	[44]
C ₂ H ₆ S								
<i>A</i> ₁	3098	-1.2	3132	-0.1	3186	1.6	3136	[45]
	2994	-2.3	3024	-1.3	3070	0.2	3064	[45]
	1457	0.7	1434	-0.9	1503	3.8	1447	[45]
	1339	0.1	1331	-0.4	1372	2.6	1337	[45]
	1031	0.1	1032	0.2	1057	2.5	1030	[45]
	680	-2.2	760	9.4	726	4.3	695	[45]
	275	-1.8	263	-6.1	264	-5.7	280	[45]
<i>B</i> ₁	3098	-1.2	3129	-0.3	3187	1.6	3137	[45]
	2997	-2.0	3016	-1.4	3076	0.6	3058	[45]
	1452	0.7	1426	-1.1	1495	3.6	1442	[45]
	1313	-0.2	1306	-0.7	1347	2.4	1315	[45]
	900	-0.3	894	-1.0	922	2.2	903	[45]
	725	-2.3	708	-4.6	779	5.0	742	[45]

Table S1 continued.

Mol	HCTH-93	$\Delta_{\text{HCTH-93}}$	1/4	$\Delta_{1/4}$	MP2	Δ_{MP2}	Expt.	Ref.
A_2	3084	-0.8	3104	-0.2	3171	2.0	3109	[45]
	1438	0.8	1450	1.6	1479	3.4	1427	[25]
	945	-0.1	933	-1.4	964	2.0	946	[45]
	176	0.0	188	7.4	181	3.4	175	[45]
B_2	3075	-1.1	3093	-0.5	3162	1.7	3109	[45]
	1449	0.7	1443	0.3	1488	3.4	1439	[45]
	976	0.3	971	-0.2	999	2.7	973	[45]
	225	23.0	183	0.0	193	5.5	183	[45]
Cl ₂ S								
A_1	506	-2.3	509	-1.7	544	5.0	518	[46]
	198	-4.8	200	-3.8	209	0.5	208	[46]
B_2	490	-6.8	522	-0.8	541	2.9	526	[46]
Cl ₂ S ₂								
A	571	4.6	587	7.5	548	0.4	546	[46]
	417	-10.5	437	-6.2	493	5.8	466	[46]
	205	1.5	207	2.5	208	3.0	202	[46]
	97	5.4	97	5.4	95	3.3	92	[46]
B	401	-12.2	421	-7.9	482	5.5	457	[46]
	229	-4.6	233	-2.9	245	2.1	240	[46]
F ₂ SO								
A'	1303	-2.2	1319	-1.1	1365	2.4	1333	[47]
	756	-6.4	776	-4.0	810	0.2	808	[47]
	485	-8.5	490	-7.5	520	-1.9	530	[47]
	331		336		368			
A''	695	-6.1	717	-3.1	749	1.2	740	[47]
	367	-5.9	368	-5.6	386	-1.0	390	[47]

Table S1 continued.

Mol	HCTH-93	$\Delta_{\text{HCTH-93}}$	1/4	$\Delta_{1/4}$	MP2	Δ_{MP2}	Expt.	Ref.
F_2S_2								
<i>A</i>	674	-6.0	695	-3.1	745	3.9	717	[48]
	628	2.1	656	6.7	621	1.0	615	[48]
	285	-10.9	287	-10.3	294	-8.1	320	[48]
	176	-3.8	178	-2.7	187	2.2	183	[48]
<i>B</i>	637	-6.5	647	-5.0	711	4.4	681	[48]
	303	0.7	306	1.7	325	8.0	301	[48]
H_2S_2								
<i>A</i>	2582	-1.5	2613	-0.3	2733	4.3	2621	[46]
	881	0.1	880	-0.2	906	2.6	882	[46]
	503	-1.2	521	2.4	537	5.5	509	[46]
	446		452		442			
<i>B</i>	2586	-3.1	2618	-1.9	2735	2.5	2669	[46]
	883	1.7	879	1.3	903	4.0	868	[46]
SO_3								
<i>A</i> ₁	1024	-3.8	1042	-2.2	1049	-1.5	1065	[49]
	465	-6.6	470	-5.6	485	-2.6	498	[49]
<i>E</i>	1352	-2.8	1375	-1.2	1409	1.3	1391	[49]
	499	-5.8	500	-5.7	514	-3.0	530	[49]
CH_2S								
<i>A</i> ₁	3012		3039		3113			
	1462		1458		1504			
	1079		1099		1100			
<i>B</i> ₁	999		999		1024			
<i>B</i> ₂	3093		3123		3209			
	987		985		1014			

Table S1 continued.

Mol	HCTH-93	$\Delta_{\text{HCTH-93}}$	1/4	$\Delta_{1/4}$	MP2	Δ_{MP2}	Expt.	Ref.
F ₂ S								
<i>A</i> ₁	806	-3.9	825	-1.7	856	2.0	839	[50]
	329	-7.8	332	-7.0	351	-1.7	357	[50]
<i>B</i> ₂	782	-3.8	802	-1.4	832	2.3	813	[50]
H ₃ NS								
<i>A</i> '	3477		3482		3588			
	3388		3399		3469			
	1634		1617		1665			
	1314		1303		1338			
	839		835		858			
	608		634		656			
<i>A</i> ''	3477		3482		3588			
	1634		1617		1665			
	839		835		858			
H ₃ PS								
<i>A</i> '	2342	-0.7	2368	0.4	2499	5.9	2359	[51]
	2321		2347		2488			
	1100	-11.3	1095	-11.7	1155	-6.9	1240	[51]
	1075		1072		1147			
	701		700		741			
	670	-21.9	685	-20.2	693	-18.8	858	[51]
<i>A</i> ''	2321	-2.1	2347	-1.0	2488	4.9	2371	[51]
	1075	-5.9	1072	-6.2	1148	0.4	1143	[51]
	701	-37.1	700	-37.2	741	-33.5	1114	[51]

Table S1 continued.

Mol	HCTH-93	$\Delta_{\text{HCTH-93}}$	1/4	$\Delta_{1/4}$	MP2	Δ_{MP2}	Expt.	Ref.
HSF								
	2603	-0.9	2627	0.0	2748	4.6	2628	[52]
	994	-2.8	995	-2.7	1043	2.0	1023	[53]
	769	-2.4	788	0.0	811	2.9	788	[53]
HSOH								
	3755	6.5	3766	6.8	3830	8.7	3525	[54]
	2556		2582		2712			
	1196	1.6	1185	0.7	1219	3.6	1177	[54]
	990		995		1035			
	750	-1.7	773	1.3	788	3.3	763	[54]
	485	9.0	489	9.9	485	9.0	445	[54]
FSOH								
	3692		3698		3787			
	1194		1180		1219			
	843		838		867			
	738		757		793			
	573		582		574			
	327		334		351			
FSOF								
	1118		1127		1369			
	761		777		813			
	431		450		519			
	397		406		421			
	289		298		241			
	158		163		138			

Table S1 continued.

Mol	HCTH-93	$\Delta_{\text{HCTH-93}}$	1/4	$\Delta_{1/4}$	MP2	Δ_{MP2}	Expt.	Ref.
CISSH								
	2545		2567		2707			
	879		880		906			
	517		535		540			
	436		455		504			
	427		429		406			
	198		200		208			