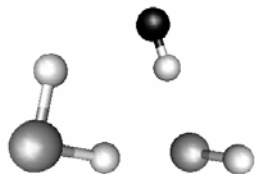


## Trimer Structures: $F^-(H_2S)_2$



$C_1$  symmetry, minimum.

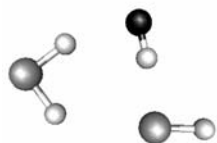
HF-SH<sup>-</sup> unit

	$r(H_b-F)$	$r(S-H_b)$	$r(S-H_t)$	$\theta(S-H_b-F)$	$\theta(H-S-H)$	$zpe$	$E_{MP2}$	$E_{e/BSSE}$	$\Delta E_{e/BSSE/Corr}$
<i>pvdz</i>	0.983	1.995	1.354	176.8	94.2	22.1	-897.459371	-897.454428	0.0
<i>pvtz</i>	0.981	1.980	1.340	176.7	93.5	22.5	-897.653025	-897.649761	0.0

SH<sub>2</sub> bound to F and S

	$r(H...F)$	$r(H...S)$	$r(S-H_F)$	$r(S-H_S)$	$\theta(H-S-H)$
<i>pvdz</i>	2.763	2.246	1.351	1.394	90.8
<i>pvtz</i>	2.631	2.239	1.338	1.382	90.4

	<i>MP2/aug-cc-pvtz</i>
$\omega_1 a$	2921 <b>2397</b>
$\omega_2 a$	2767 <b>4</b>
$\omega_3 a$	2744 <b>25</b>
$\omega_4 a$	2214 <b>1709</b>
$\omega_5 a$	1189 <b>37</b>
$\omega_6 a$	954 <b>21</b>
$\omega_7 a$	887 <b>52</b>
$\omega_8 a$	599 <b>&lt;1</b>
$\omega_9 a$	309 <b>15</b>
$\omega_{10} a$	299 <b>5</b>
$\omega_{11} a$	245 <b>27</b>
$\omega_{12} a$	220 <b>9</b>
$\omega_{13} a$	172 <b>10</b>
$\omega_{14} a$	132 <b>35</b>
$\omega_{15} a$	49 <b>1</b>



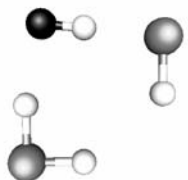
$C_s$  symmetry, 1 imaginary frequency ( $a''$ )

HF-SH unit

	$r(H_b-F)$	$r(S-H_b)$	$r(S-H_d)$	$\theta(S-H_b-F)$	$\theta(H-S-H)$	$zpe$	$E_{MP2}$	$E_{e/BSSE}$	$\Delta E_{e/BSSE/Corr}$
<i>pvdz</i>	1.004	1.920	1.352	173.9	98.2	21.8	-897.454722	-897.450330	2.3
<i>pvtz</i>	0.997	1.921	1.339	174.1	97.5	22.1	-897.648509	-897.645473	2.3

SH<sub>2</sub> bound to F and S

	$r(H...F)$	$r(H...S)$	$r(S-H_F)$	$r(S-H_S)$	$\theta(H-S-H)$
<i>pvdz</i>	2.107	2.765	1.357	1.353	90.6
<i>pvtz</i>	2.134	2.665	1.344	1.341	90.5



$C_s$  symmetry, 1 imaginary frequency ( $a''$ )

HF-SH unit

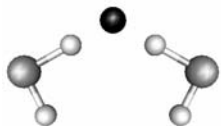
	$r(H_b-F)$	$r(S-H_b)$	$r(S-H_d)$	$\theta(S-H_b-F)$	$\theta(H-S-H)$	$zpe$	$E_{MP2}$	$E_{e/BSSE}$	$\Delta E_{e/BSSE/Corr}$
<i>pvdz</i>	1.019	1.877	1.354	178.4	95.4	21.5	-897.453961	-897.449466	2.5
<i>pvtz</i>	1.009	1.884	1.340	178.8	95.6	21.9	-897.647509	-897.644450	2.7

SH<sub>2</sub> bound to F

	$r(H...F)$	$r(S-H_F)$	$r(S-H_H)$	$\theta(H-S-H)$
<i>pvdz</i>	1.918	1.364	1.350	91.4
<i>pvtz</i>	1.941	1.350	1.337	91.0

	<i>MP2/aug-cc-pvtz</i>
$\omega_1 a'$	2747 <b>66</b>
$\omega_2 a'$	2736 <b>354</b>
$\omega_3 a'$	2722 <b>335</b>
$\omega_4 a'$	2615 <b>2303</b>
$\omega_5 a'$	1204 <b>12</b>
$\omega_6 a'$	1049 <b>51</b>
$\omega_7 a'$	308 <b>8</b>
$\omega_8 a'$	272 <b>17</b>
$\omega_9 a'$	181 <b>24</b>
$\omega_{10} a'$	118 <b>17</b>
$\omega_{11} a'$	58 <b>5</b>
$\omega_{12} a''$	890 <b>16</b>
$\omega_{13} a''$	348 <b>4</b>
$\omega_{14} a''$	199 <b>1</b>
$\omega_{15} a''$	207i <b>15</b>

	<i>MP2/aug-cc-pvtz</i>
$\omega_1 a'$	2774 <b>8</b>
$\omega_2 a'$	2737 <b>48</b>
$\omega_3 a'$	2646 <b>494</b>
$\omega_4 a'$	2411 <b>3120</b>
$\omega_5 a'$	1214 <b>7</b>
$\omega_6 a'$	1080 <b>40</b>
$\omega_7 a'$	354 <b>17</b>
$\omega_8 a'$	291 <b>28</b>
$\omega_9 a'$	176 <b>22</b>
$\omega_{10} a'$	133 <b>21</b>
$\omega_{11} a'$	45 <b>3</b>
$\omega_{12} a''$	913 <b>15</b>
$\omega_{13} a''$	411 <b>6</b>
$\omega_{14} a''$	130 <b>5</b>
$\omega_{15} a''$	159i <b>&lt;1</b>



$C_{2v}$  symmetry, 2 imaginary frequencies ( $a_2$ ,  $b_2$ )

	$r(F-H_b)$	$r(S-H_b)$	$r(S-H_l)$	$\theta(F-H_b-S)$	$\theta(H-S-H)$	$\theta(H_b-F-H_b)$	$zpe$	$E_{MP2}$	$E_e/BSSE$	$\Delta E_e/BSSE/Corr$
<i>pvdz</i>	1.389	1.476	1.350	179.2	93.4	114.5	19.4	-897.449915	-897.444198	3.7
<i>pvtz</i>	1.355	1.477	1.337	179.0	93.2	118.8	19.1	-897.641292	-897.637592	4.3



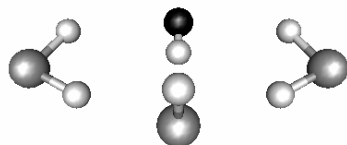
$C_{2v}$  symmetry, 3 imaginary frequencies ( $a_2$ ,  $b_1$ ,  $b_2$ )

	$r(F-H_b)$	$r(S-H_b)$	$r(S-H_l)$	$\theta(F-H_b-S)$	$\theta(H-S-H)$	$\theta(H_b-F-H_b)$	$zpe$	$E_{MP2}$	$E_e/BSSE$	$\Delta E_e/BSSE/Corr$
<i>pvdz</i>	1.394	1.472	1.350	178.4	93.5	130.9	19.3	-897.449284	-897.443759	3.9
<i>pvtz</i>	1.365	1.471	1.337	178.4	93.3	136.6	19.1	-897.640741	-897.637125	4.6

	<i>MP2/aug-cc-pvtz</i>
$\omega_1 a_1$	2770 <b>13</b>
$\omega_2 a_1$	1578 <b>1222</b>
$\omega_3 a_1$	1274 <b>20</b>
$\omega_4 a_1$	453 <b>29</b>
$\omega_5 a_1$	294 <b>36</b>
$\omega_6 a_1$	22 < <b>1</b>
$\omega_7 a_2$	856 <b>0</b>
$\omega_8 a_2$	73i <b>0</b>
$\omega_9 b_1$	856 <b>12</b>
$\omega_{10} b_1$	42 <b>11</b>
$\omega_{11} b_2$	2770 <b>4</b>
$\omega_{12} b_2$	1233 <b>14</b>
$\omega_{13} b_2$	814 <b>3151</b>
$\omega_{14} b_2$	418 <b>7</b>
$\omega_{15} b_2$	544i <b>5032</b>

	<i>MP2/aug-cc-pvtz</i>
$\omega_1 a_1$	2772 <b>16</b>
$\omega_2 a_1$	1626 <b>370</b>
$\omega_3 a_1$	1254 <b>2</b>
$\omega_4 a_1$	441 <b>10</b>
$\omega_5 a_1$	247 <b>10</b>
$\omega_6 a_1$	24 < <b>1</b>
$\omega_7 a_2$	854 <b>0</b>
$\omega_8 a_2$	47i <b>0</b>
$\omega_9 b_1$	831 <b>13</b>
$\omega_{10} b_1$	24i <b>16</b>
$\omega_{11} b_2$	2772 <b>3</b>
$\omega_{12} b_2$	1242 <b>115</b>
$\omega_{13} b_2$	877 <b>4627</b>
$\omega_{14} b_2$	422 <b>34</b>
$\omega_{15} b_2$	512i <b>5987</b>

## Tetramer Structures: F<sup>-</sup>-(H<sub>2</sub>S)<sub>3</sub>



C<sub>s</sub> symmetry, minimum

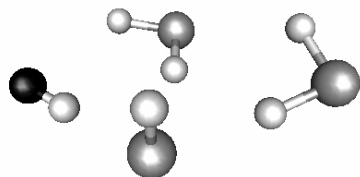
HF-SH<sup>-</sup> unit

	$r(\text{F-H}_b)$	$r(\text{S-H}_b)$	$r(\text{S-H})$	$\theta(\text{F-H}_b\text{-S})$	$\theta(\text{H-S-H})$	$zpe$	$E_{MP2}$	$E_{e/BSSE}$	$\Delta E_{e/BSSE}$	$\Delta E_{e/BSSE/Corr}$
<i>pvdz</i>	0.982	1.994	1.354	179.6	93.6	33.0	-1296.329537	-1296.322323	0.0	0.0
<i>pvtz</i>	0.980	1.978	1.340	179.8	92.8	33.4	-1296.578488	-1296.574028	0.0	0.0

SH<sub>2</sub> bound to F and S

	$r(\text{H}\dots\text{F})$	$r(\text{H}\dots\text{S})$	$r(\text{S-H}_F)$	$r(\text{S-H}_S)$	$\theta(\text{H-S-H})$
<i>pvdz</i>	2.690	2.341	1.351	1.380	90.8
<i>pvtz</i>	2.587	2.330	1.338	1.368	90.5

	<i>MP2/aug-cc-pvtz</i>
$\omega_1 a'$	2927 <b>2006</b>
$\omega_2 a'$	2767 <b>4</b>
$\omega_3 a'$	2746 <b>14</b>
$\omega_4 a'$	2399 <b>170</b>
$\omega_5 a'$	1193 <b>20</b>
$\omega_6 a'$	935 <b>16</b>
$\omega_7 a'$	514 <b>2</b>
$\omega_8 a'$	315 <b>17</b>
$\omega_9 a'$	273 <b>1</b>
$\omega_{10} a'$	238 <b>8</b>
$\omega_{11} a'$	210 <b>11</b>
$\omega_{12} a'$	101 <b>3</b>
$\omega_{13} a'$	36 <b>1</b>
$\omega_{14} a'$	18 <b>1</b>
$\omega_{15} a''$	2768 <b>6</b>
$\omega_{16} a''$	2361 <b>2204</b>
$\omega_{17} a''$	1197 <b>26</b>
$\omega_{18} a''$	907 <b>79</b>
$\omega_{19} a''$	547 <b>&lt;1</b>
$\omega_{20} a''$	268 <b>5</b>
$\omega_{21} a''$	242 <b>28</b>
$\omega_{22} a''$	185 <b>8</b>
$\omega_{23} a''$	138 <b>56</b>
$\omega_{24} a''$	65 <b>&lt;1</b>



$C_1$  symmetry, minimum

HF-SH<sup>-</sup> unit

	$r(\text{F-H}_b)$	$r(\text{S-H}_b)$	$r(\text{S-H}_l)$	$\theta(\text{F-H}_b\text{-S})$	$\theta(\text{H-S-H})$	$zpe$	$E_{\text{MP2}}$	$E_{e/\text{BSSE}}$	$\Delta E_{e/\text{BSSE}}$	$\Delta E_{e/\text{BSSE}/\text{Corr}}$
<i>pvdz</i>	0.976	2.024	1.354	177.0	92.0	33.1	-1296.329437	-1296.321831	0.3	0.4
<i>pvtz</i>	0.973	2.009	1.340	177.1	91.7	33.4	-1296.578410	-1296.573807	0.1	0.1

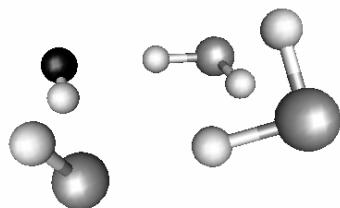
SH<sub>2</sub> bound to F and S

	$r(\text{H}\dots\text{F})$	$r(\text{H}\dots\text{S})$	$r(\text{S-H}_F)$	$r(\text{S-H}_S)$	$\theta(\text{H-S-H})$
<i>pvdz</i>	2.690	2.321	1.351	1.382	90.8
<i>pvtz</i>	2.636	2.299	1.338	1.371	90.7

SH<sub>2</sub> bound to SH<sup>-</sup> and SH<sub>2</sub> only

	$r(\text{H}\dots\text{S})$	$r(\text{H}\dots\text{SH}_2)$	$r(\text{S-H}_S)$	$r(\text{S-H}_l)$	$\theta(\text{H-S-H})$
<i>pvdz</i>	2.306	3.008	1.384	1.351	92.0
<i>pvtz</i>	2.288	2.967	1.372	1.338	91.8

	<i>MP2/aug-cc-pvtz</i>
$\omega_1 a$	3061 <b>2192</b>
$\omega_2 a$	2767 <b>2</b>
$\omega_3 a$	2763 <b>1</b>
$\omega_4 a$	2745 <b>12</b>
$\omega_5 a$	2360 <b>1636</b>
$\omega_6 a$	2294 <b>855</b>
$\omega_7 a$	1211 <b>5</b>
$\omega_8 a$	1192 <b>16</b>
$\omega_9 a$	914 <b>27</b>
$\omega_{10} a$	854 <b>42</b>
$\omega_{11} a$	567 <b>2</b>
$\omega_{12} a$	535 <b>1</b>
$\omega_{13} a$	320 <b>16</b>
$\omega_{14} a$	305 <b>2</b>
$\omega_{15} a$	302 <b>8</b>
$\omega_{16} a$	239 <b>24</b>
$\omega_{17} a$	230 <b>25</b>
$\omega_{18} a$	195 <b>6</b>
$\omega_{19} a$	165 <b>7</b>
$\omega_{20} a$	144 <b>38</b>
$\omega_{21} a$	99 <b>10</b>
$\omega_{22} a$	56 <b>2</b>
$\omega_{23} a$	53 <b>1</b>
$\omega_{24} a$	23 <b>&lt;1</b>



$C_1$  symmetry, minimum

HF-SH unit

	$r(F-H_b)$	$r(S-H_b)$	$r(S-H_f)$	$\theta(F-H_b-S)$	$\theta(H-S-H)$	$zpe$	$E_{MP2}$	$E_{e/BSSE}$	$\Delta E_{e/BSSE}$	$\Delta E_{e/BSSE/Corr}$
<i>pvdz</i>	0.995	1.943	1.353	176.7	95.9	32.9	-1296.327756	-1296.320285	1.3	1.2
<i>pvtz</i>	0.988	1.940	1.339	176.5	95.3	33.2	-1296.576599	-1296.571875	1.4	1.2

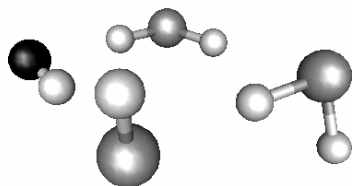
SH<sub>2</sub> bound to F and S

	$r(H...F)$	$r(H...S)$	$r(S-H_F)$	$r(S-H_S)$	$\theta(H-S-H)$
<i>pvdz</i>	2.049	2.723	1.358	1.355	92.5
<i>pvtz</i>	2.056	2.725	1.345	1.342	92.4

SH<sub>2</sub> bound to S only

	$r(H...S)$	$r(S-H_S)$	$r(S-H_f)$	$\theta(H-S-H)$
<i>pvdz</i>	2.156	1.410	1.350	92.5
<i>pvtz</i>	2.140	1.399	1.337	92.2

	<i>MP2/aug-cc-pvtz</i>
$\omega_1 a$	2813 <b>2286</b>
$\omega_2 a$	2272 <b>2</b>
$\omega_3 a$	2746 <b>34</b>
$\omega_4 a$	2712 <b>33</b>
$\omega_5 a$	2669 <b>553</b>
$\omega_6 a$	2005 <b>2555</b>
$\omega_7 a$	1216 <b>1</b>
$\omega_8 a$	1197 <b>8</b>
$\omega_9 a$	988 <b>29</b>
$\omega_{10} a$	898 <b>28</b>
$\omega_{11} a$	664 <b>4</b>
$\omega_{12} a$	370 <b>6</b>
$\omega_{13} a$	339 <b>7</b>
$\omega_{14} a$	329 <b>2</b>
$\omega_{15} a$	318 <b>8</b>
$\omega_{16} a$	265 <b>14</b>
$\omega_{17} a$	225 <b>16</b>
$\omega_{18} a$	215 <b>16</b>
$\omega_{19} a$	146 <b>59</b>
$\omega_{20} a$	124 <b>28</b>
$\omega_{21} a$	104 <b>2</b>
$\omega_{22} a$	72 <b>3</b>
$\omega_{23} a$	24 <b>1</b>
$\omega_{24} a$	16 <b>&lt;1</b>



$C_1$  symmetry, minimum

HF-SH unit

	$r(F-H_b)$	$r(S-H_b)$	$r(S-H_d)$	$\theta(F-H_b-S)$	$\theta(H-S-H)$	$zpe$	$E_{MP2}$	$E_{e/BSSE}$	$\Delta E_{e/BSSE}$	$\Delta E_{e/BSSE/Corr}$
<i>pvdz</i>	0.992	1.949	1.353	177.2	96.2	32.9	-1296.327421	-1296.319956	1.5	1.4
<i>pvtz</i>	0.986	1.946	1.339	176.7	95.8	33.1	-1296.576163	-1296.571458	1.6	1.3

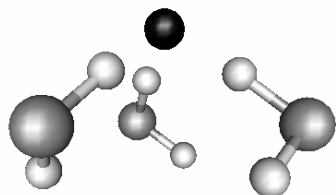
SH<sub>2</sub> bound to F and SH<sub>2</sub>

	$r(H...F)$	$r(H...SH_2)$	$r(S-H_F)$	$r(S-H_{SH_2})$	$\theta(H-S-H)$
<i>pvdz</i>	2.059	2.680	1.358	1.356	92.6
<i>pvtz</i>	2.072	2.678	1.345	1.343	92.6

SH<sub>2</sub> bound to S only

	$r(H...S)$	$r(S-H_s)$	$r(S-H_t)$	$\theta(H-S-H)$
<i>pvdz</i>	2.155	1.411	1.350	92.2
<i>pvtz</i>	2.134	1.401	1.337	91.9

	<i>MP2/aug-cc-pvtz</i>
$\omega_1 a$	2841 <b>2403</b>
$\omega_2 a$	2774 <b>1</b>
$\omega_3 a$	2747 <b>26</b>
$\omega_4 a$	2701 <b>46</b>
$\omega_5 a$	2679 <b>456</b>
$\omega_6 a$	1982 <b>2696</b>
$\omega_7 a$	1217 <b>3</b>
$\omega_8 a$	1205 <b>9</b>
$\omega_9 a$	975 <b>25</b>
$\omega_{10} a$	899 <b>28</b>
$\omega_{11} a$	643 <b>5</b>
$\omega_{12} a$	367 <b>9</b>
$\omega_{13} a$	356 <b>1</b>
$\omega_{14} a$	331 <b>1</b>
$\omega_{15} a$	309 <b>11</b>
$\omega_{16} a$	264 <b>9</b>
$\omega_{17} a$	234 <b>22</b>
$\omega_{18} a$	200 <b>18</b>
$\omega_{19} a$	145 <b>64</b>
$\omega_{20} a$	112 <b>7</b>
$\omega_{21} a$	81 <b>6</b>
$\omega_{22} a$	73 <b>1</b>
$\omega_{23} a$	27 <b>1</b>
$\omega_{24} a$	13 <b>1</b>

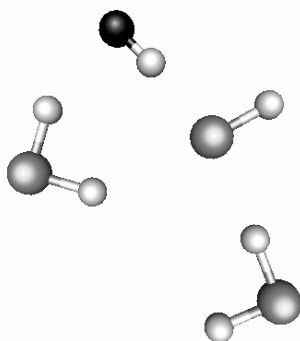


$C_3$  symmetry, minimum

	$r(F-H_b)$	$r(S-H_b)$	$r(S-H_d)$	$\theta(F-H_b-S)$	$\theta(H-S-H)$	$\theta(H_b-F-H_b)$	$zpe$	$E_{MP2}$	$E_{e/BSSE}$	$\Delta E_{e/BSSE}$	$\Delta E_{e/BSSE/Corr}$
<i>pvdz</i>	1.575	1.411	1.351	174.5	91.7	94.9	32.0	-1296.323346	-1296.315493	4.3	3.3
<i>pvtz</i>	1.571	1.400	1.338	174.0	91.5	94.5	31.9	-1296.569060	-1296.564323	6.0	4.6

	<i>MP2/aug-cc-pvtz</i>
$\omega_1 a$	2767 <1
$\omega_2 a$	2220 <b>880</b>
$\omega_3 a$	1233 <b>4</b>
$\omega_4 a$	711 <b>6</b>
$\omega_5 a$	378 <b>19</b>
$\omega_6 a$	268 <b>44</b>
$\omega_7 a$	222 <b>4</b>
$\omega_8 a$	39 <1
$\omega_9 e$	2768 <b>1 (2)</b>
$\omega_{10} e$	1874 <b>1920 (3840)</b>
$\omega_{11} e$	1233 <b>33 (66)</b>
$\omega_{12} e$	720 <b>30 (60)</b>
$\omega_{13} e$	366 <b>12 (24)</b>
$\omega_{14} e$	140 <b>9 (18)</b>
$\omega_{15} e$	124 <b>156 (312)</b>
$\omega_{16} e$	28 <b>5 (10)</b>





$C_s$  symmetry, 3 imaginary frequencies ( $3a''$ )

HF-SH<sup>-</sup> unit

	$r(H_b-F)$	$r(S-H_b)$	$r(S-H_t)$	$\theta(S-H_b-F)$	$\theta(H-S-H)$	$zpe$	$E_{MP2}$	$E_{e/BSSE}$	$\Delta E_{e/BSSE}$	$\Delta E_{e/BSSE/Corr}$
<i>pvdz</i>	0.985	1.972	1.350	172.0	104.1	32.4	-1296.323138	-1296.316558	3.6	3.0
<i>pvtz</i>	0.982	1.964	1.339	173.8	100.0	32.6	-1296.572455	-1296.568387	3.5	2.7

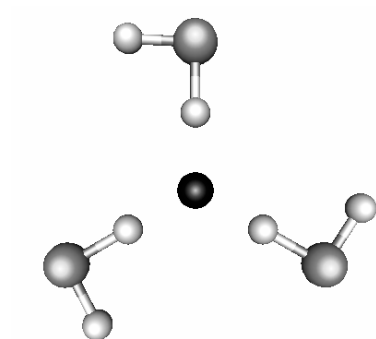
SH<sub>2</sub> bound to H-F and SH<sup>-</sup>

	$r(H...F)$	$r(H...S)$	$r(S-H_F)$	$r(S-H_S)$	$\theta(H-S-H)$
<i>pvdz</i>	2.204	2.692	1.355	1.353	90.8
<i>pvtz</i>	2.175	2.686	1.342	1.341	90.7

SH<sub>2</sub> bound to SH<sup>-</sup>

	$r(H...S)$	$r(S-H_S)$	$r(S-H_t)$	$\theta(H-S-H)$
<i>pvdz</i>	2.303	1.384	1.350	92.4
<i>pvtz</i>	2.267	1.375	1.336	92.3

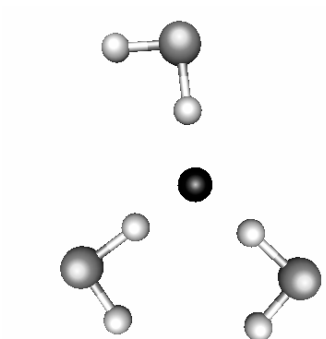
	<i>MP2/aug-cc-pvtz</i>
$\omega_1 a'$	2908 <b>2655</b>
$\omega_2 a'$	2778 <b>2</b>
$\omega_3 a'$	2751 <b>40</b>
$\omega_4 a'$	2739 <b>17</b>
$\omega_5 a'$	2716 <b>130</b>
$\omega_6 a'$	2289 <b>2047</b>
$\omega_7 a'$	1220 <b>4</b>
$\omega_8 a'$	1205 <b>10</b>
$\omega_9 a'$	987 <b>52</b>
$\omega_{10} a'$	369 <b>6</b>
$\omega_{11} a'$	272 <b>16</b>
$\omega_{12} a'$	255 <b>31</b>
$\omega_{13} a'$	180 <b>35</b>
$\omega_{14} a'$	119 <b>22</b>
$\omega_{15} a'$	107 <b>10</b>
$\omega_{16} a'$	64 <b>2</b>
$\omega_{17} a'$	11 <1
$\omega_{18} a''$	831 <b>26</b>
$\omega_{19} a''$	481 <b>2</b>
$\omega_{20} a''$	323 <b>4</b>
$\omega_{21} a''$	177 <b>1</b>
$\omega_{22} a''$	26i <b>1</b>
$\omega_{23} a''$	91i <b>6</b>
$\omega_{24} a''$	214i <b>17</b>



$C_{3h}$  symmetry, 3 imaginary frequencies ( $1a' + 2e''$ )

	$r(F-H_b)$	$r(S-H_b)$	$r(S-H_t)$	$\theta(F-H_b-S)$	$\theta(H-S-H)$	$\theta(H_b-F-H_b)$	$zpe$	$E_{MP2}$	$E_{e/BSSE}$	$\Delta E_{e/BSSE}$	$\Delta E_{e/BSSE/Corr}$
<i>pvdz</i>	1.559	1.415	1.349	180.0	93.2	120.0	31.1	-1296.321644	-1296.314762	4.7	2.9
<i>pvtz</i>	1.550	1.404	1.336	179.8	93.0	120.0	31.0	-1296.567500	-1296.563317	6.7	4.3

	<i>MP2/aug-cc-pvtz</i>
$\omega_1 a'$	2778 <b>0</b>
$\omega_2 a'$	2174 <b>0</b>
$\omega_3 a'$	1228 <b>0</b>
$\omega_4 a'$	366 <b>0</b>
$\omega_5 a'$	168 <b>0</b>
$\omega_6 a''$	707 <b>14</b>
$\omega_7 a''$	25 < <b>1</b>
$\omega_8 a''$	76i <b>27</b>
$\omega_9 e'$	2778 <b>5 (10)</b>
$\omega_{10} e'$	1825 <b>3693 (7386)</b>
$\omega_{11} e'$	1253 <b>4 (8)</b>
$\omega_{12} e'$	390 <b>48 (96)</b>
$\omega_{13} e'$	160 <b>340 (680)</b>
$\omega_{14} e'$	10 < <b>1 (1)</b>
$\omega_{15} e''$	690 <b>0</b>
$\omega_{16} e''$	21i <b>0</b>



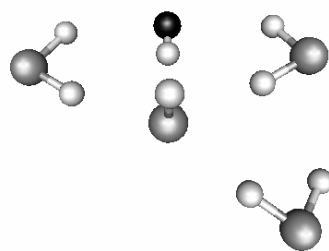
$C_S$  symmetry, 2 imaginary frequencies ( $2a''$ )

	$r(F-H_b)$	$r(S-H_b)$	$r(S-H_l)$	$\theta(F-H_b-S)$	$\theta(H-S-H)$	$\theta(H_b-F-H_b)$	$zpe$	$E_{MP2}$	$E_e/BSSE$	$\Delta E_e/BSSE$	$\Delta E_e/BSSE/Corr$
<i>pvdz</i>	1.570 <i>t</i>	1.411	1.349	179.3	93.2	137.4 ( <i>t-r</i> )	31.2	-1296.321748	-1296.314697	4.8	3.0
	1.562 <i>r</i>	1.414	1.350	177.9	93.0	104.1 ( <i>r-l</i> )					
	1.545 <i>l</i>	1.419	1.350	178.8	93.1	118.5 ( <i>l-t</i> )					
<i>pvtz</i>	1.558 <i>t</i>	1.402	1.336	179.2	92.9	136.9 ( <i>t-r</i> )	31.0	-1296.567592	-1296.563343	6.7	4.3
	1.553 <i>r</i>	1.403	1.336	177.9	92.9	103.4 ( <i>r-l</i> )					
	1.539 <i>l</i>	1.408	1.337	178.7	92.9	119.7 ( <i>l-t</i> )					

*t*=top, *r*=right, *l*=left

	<i>MP2/aug-cc-pvtz</i>
$\omega_1 a'$	2778 4
$\omega_2 a'$	2776 5
$\omega_3 a'$	2775 4
$\omega_4 a'$	2180 13
$\omega_5 a'$	1852 4599
$\omega_6 a'$	1793 2613
$\omega_7 a'$	1261 5
$\omega_8 a'$	1246 1
$\omega_9 a'$	1227 4
$\omega_{10} a'$	404 65
$\omega_{11} a'$	382 29
$\omega_{12} a'$	360 1
$\omega_{13} a'$	193 312
$\omega_{14} a'$	164 196
$\omega_{15} a'$	131 179
$\omega_{16} a'$	23 <1
$\omega_{17} a'$	13 <1
$\omega_{18} a''$	712 10
$\omega_{19} a''$	686 1
$\omega_{20} a''$	682 2
$\omega_{21} a''$	50 7
$\omega_{22} a''$	23 <1
$\omega_{23} a''$	32i 15
$\omega_{24} a''$	119i <1

## Pentamer Structures: F<sup>-</sup>-(H<sub>2</sub>S)<sub>4</sub>



*C*<sub>1</sub> symmetry, minimum

FH...SH<sup>-</sup> core

	<i>r</i> (F-H <sub>b</sub> )	<i>r</i> (S-H <sub>b</sub> )	<i>r</i> (S-H <sub>l</sub> )	∠(F-H <sub>b</sub> -S)	∠(H-S-H)	<i>zpe</i>	<i>E</i> <sub>MP2</sub>	<i>E</i> <sub><i>e</i>/BSSE</sub>	Δ <i>E</i> <sub><i>e</i>/BSSE</sub>	Δ <i>E</i> <sub><i>e</i>/BSSE/Corr</sub>
<i>pvdz</i>	0.976	2.013	1.353	178.8	96.4	44.0	-1695.198223	-1695.188495	0.0	0.0

Bottom SH<sub>2</sub> bound to SH<sup>-</sup> and SH<sub>2</sub>

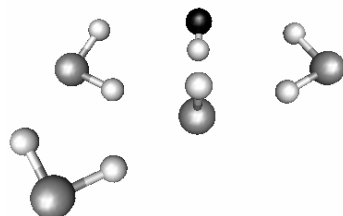
	<i>r</i> (H...S)	<i>r</i> (H...SH <sub>2</sub> )	<i>r</i> (S-H <sub>SH<sup>-</sup></sub> )	<i>r</i> (S-H <sub>SH<sub>2</sub></sub> )	∠(H-S-H)
<i>pvdz</i>	2.373	2.979	1.375	1.351	91.8

SH<sub>2</sub>'s bound to core

	<i>r</i> (H...F)	<i>r</i> (H...S)	<i>r</i> (S-H <sub><i>r</i></sub> )	<i>r</i> (S-H <sub><i>s</i></sub> )	∠(H-S-H)
<i>pvdz</i>	2.714 <i>r</i>	2.365	1.351	1.377	90.9
	2.628 <i>l</i>	2.407	1.351	1.373	90.8

*r*=right, *l*=left

	<i>MP2/aug-cc-pvdz</i>
<b>ω<sub>1</sub> <i>a</i></b>	2973 <b>1830</b>
<b>ω<sub>2</sub> <i>a</i></b>	2754 <b>2</b>
<b>ω<sub>3</sub> <i>a</i></b>	2752 <b>1</b>
<b>ω<sub>4</sub> <i>a</i></b>	2747 <b>1</b>
<b>ω<sub>5</sub> <i>a</i></b>	2728 <b>10</b>
<b>ω<sub>6</sub> <i>a</i></b>	2481 <b>80</b>
<b>ω<sub>7</sub> <i>a</i></b>	2442 <b>2205</b>
<b>ω<sub>8</sub> <i>a</i></b>	2402 <b>614</b>
<b>ω<sub>9</sub> <i>a</i></b>	1198 <b>3</b>
<b>ω<sub>10</sub> <i>a</i></b>	1185 <b>25</b>
<b>ω<sub>11</sub> <i>a</i></b>	1181 <b>9</b>
<b>ω<sub>12</sub> <i>a</i></b>	898 <b>22</b>
<b>ω<sub>13</sub> <i>a</i></b>	859 <b>70</b>
<b>ω<sub>14</sub> <i>a</i></b>	535 <b>3</b>
<b>ω<sub>15</sub> <i>a</i></b>	502 <b>3</b>
<b>ω<sub>16</sub> <i>a</i></b>	478 <b>4</b>
<b>ω<sub>17</sub> <i>a</i></b>	323 <b>10</b>
<b>ω<sub>18</sub> <i>a</i></b>	286 <b>4</b>
<b>ω<sub>19</sub> <i>a</i></b>	271 <b>7</b>
<b>ω<sub>20</sub> <i>a</i></b>	252 <b>15</b>
<b>ω<sub>21</sub> <i>a</i></b>	242 <b>2</b>
<b>ω<sub>22</sub> <i>a</i></b>	230 <b>32</b>
<b>ω<sub>23</sub> <i>a</i></b>	215 <b>13</b>
<b>ω<sub>24</sub> <i>a</i></b>	193 <b>5</b>
<b>ω<sub>25</sub> <i>a</i></b>	164 <b>5</b>
<b>ω<sub>26</sub> <i>a</i></b>	146 <b>60</b>
<b>ω<sub>27</sub> <i>a</i></b>	96 <b>7</b>
<b>ω<sub>28</sub> <i>a</i></b>	93 <b>1</b>
<b>ω<sub>29</sub> <i>a</i></b>	58 < <b>1</b>
<b>ω<sub>30</sub> <i>a</i></b>	55 <b>1</b>
<b>ω<sub>31</sub> <i>a</i></b>	29 <b>1</b>
<b>ω<sub>32</sub> <i>a</i></b>	22 < <b>1</b>
<b>ω<sub>33</sub> <i>a</i></b>	17 <b>1</b>



$C_1$  symmetry, minimum

FH...SH<sup>-</sup> core

	$r(F-H_b)$	$r(S-H_b)$	$r(S-H_l)$	$\theta(F-H_b-S)$	$\theta(H-S-H)$	$zpe$	$E_{MP2}$	$E_{e/BSSE}$	$\Delta E_{e/BSSE}$	$\Delta E_{e/BSSE/Corr}$
<i>pvdz</i>	0.976	2.018	1.354	179.1	91.8	44.0	-1695.197936	-1695.188245	0.2	0.2

Bottom SH<sub>2</sub> bound to SH

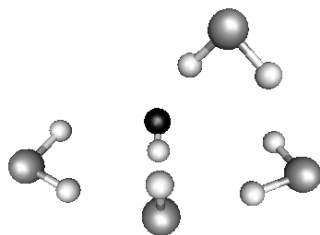
	$r(H...S)$	$r(S-H_{SH})$	$r(S-H_l)$	$\theta(H-S-H)$
<i>pvdz</i>	2.362	1.377	1.351	91.9

SH<sub>2</sub>'s bound to core

	$r(H...F)$	$r(H...S)$	$r(S-H_r)$	$r(S-H_l)$	$\theta(H-S-H)$
<i>pvdz</i>	2.628 <i>r</i>	2.404	1.351	1.373	90.8
	2.750 <i>l</i>	2.366	1.351	1.376	91.0

*r*=right, *l*=left

	<i>MP2/aug-cc-pvdz</i>
$\omega_1 a$	2982 1851
$\omega_2 a$	2754 2
$\omega_3 a$	2753 1
$\omega_4 a$	2749 <1
$\omega_5 a$	2724 10
$\omega_6 a$	2478 113
$\omega_7 a$	2433 2335
$\omega_8 a$	2400 560
$\omega_9 a$	1200 3
$\omega_{10} a$	1185 28
$\omega_{11} a$	1182 8
$\omega_{12} a$	888 23
$\omega_{13} a$	856 67
$\omega_{14} a$	541 2
$\omega_{15} a$	497 <1
$\omega_{16} a$	473 6
$\omega_{17} a$	325 19
$\omega_{18} a$	290 14
$\omega_{19} a$	275 2
$\omega_{20} a$	250 6
$\omega_{21} a$	245 4
$\omega_{22} a$	230 37
$\omega_{23} a$	204 16
$\omega_{24} a$	191 2
$\omega_{25} a$	159 5
$\omega_{26} a$	147 64
$\omega_{27} a$	95 5
$\omega_{28} a$	91 2
$\omega_{29} a$	57 <1
$\omega_{30} a$	52 1
$\omega_{31} a$	29 1
$\omega_{32} a$	22 <1
$\omega_{33} a$	17 1



$C_1$  symmetry, minimum

	$r(F-H_b)$	$r(S-H_b)$	$r(S-H_l)$	$\theta(F-H_b-S)$	$\theta(H-S-H)$	$zpe$	$E_{MP2}$	$E_{e/BSSE}$	$\Delta E_{e/BSSE}$	$\Delta E_{e/BSSE/Corr}$
<i>pvdz</i>	0.997	1.932	1.354	177.5	92.1	43.8	-1695.196611	-1695.186646	1.2	1.0

Top  $SH_2$  bound to F and  $SH_2$

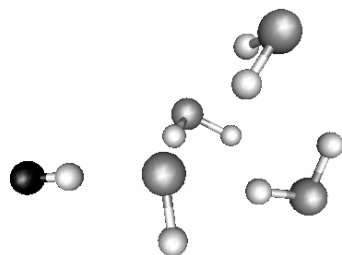
	$r(H...F)$	$r(H...SH_2)$	$r(S-H_r)$	$r(S-H_s)$	$\theta(H-S-H)$
<i>pvdz</i>	2.088	2.771	1.357	1.354	91.4

$SH_2$ 's bound to core

	$r(H...F)$	$r(H...S)$	$r(S-H_r)$	$r(S-H_s)$	$\theta(H-S-H)$
<i>pvdz</i>	3.175 <i>r</i>	2.260	1.351	1.389	91.8
	2.626 <i>l</i>	2.388	1.351 <i>l</i>	1.375	90.7

*r*=right, *l*=left

	<i>MP2/aug-cc-pvdz</i>
$\omega_1 a$	2756 <b>19</b>
$\omega_2 a$	2752 <b>1</b>
$\omega_3 a$	2723 <b>19</b>
$\omega_4 a$	2715 <b>195</b>
$\omega_5 a$	2702 <b>197</b>
$\omega_6 a$	2593 <b>1982</b>
$\omega_7 a$	2436 <b>728</b>
$\omega_8 a$	2251 <b>1746</b>
$\omega_9 a$	1201 <b>4</b>
$\omega_{10} a$	1188 <b>6</b>
$\omega_{11} a$	1182 <b>16</b>
$\omega_{12} a$	997 <b>31</b>
$\omega_{13} a$	905 <b>60</b>
$\omega_{14} a$	590 <b>4</b>
$\omega_{15} a$	492 <b>3</b>
$\omega_{16} a$	366 <b>7</b>
$\omega_{17} a$	348 <b>19</b>
$\omega_{18} a$	293 <b>2</b>
$\omega_{19} a$	289 <b>12</b>
$\omega_{20} a$	272 <b>10</b>
$\omega_{21} a$	254 <b>18</b>
$\omega_{22} a$	243 <b>6</b>
$\omega_{23} a$	232 <b>16</b>
$\omega_{24} a$	191 <b>7</b>
$\omega_{25} a$	159 <b>23</b>
$\omega_{26} a$	141 <b>62</b>
$\omega_{27} a$	114 <b>5</b>
$\omega_{28} a$	97 <b>1</b>
$\omega_{29} a$	73 <b>1</b>
$\omega_{30} a$	48 <b>&lt;1</b>
$\omega_{31} a$	29 <b>1</b>
$\omega_{32} a$	16 <b>1</b>
$\omega_{33} a$	13 <b>&lt;1</b>



$C_1$  symmetry, minimum

HF-SH unit

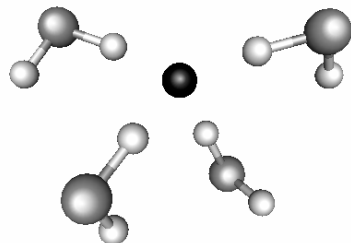
	$r(F-H_b)$	$r(S-H_b)$	$r(S-H_l)$	$\theta(F-H_b-S)$	$\theta(H-S-H)$	$zpe$	$E_{MP2}$	$E_{e/BSSE}$	$\Delta E_{e/BSSE}$	$\Delta E_{e/BSSE/Corr}$
<i>pvdz</i>	0.967	2.061	1.353	179.6	96.1	44.3	-1695.197605	-1695.186986	1.0	1.3

Other SH<sub>2</sub> units

	$r(H...S)$	$r(H...SH_2)$	$r(S-H_s)$	$r(S-H)$	$\theta(H-S-H)$
<i>pvdz</i>	2.424 <i>t</i>	2.846	1.368	1.355	90.9
	2.389 <i>r</i>	2.888	1.377	1.353	90.9
	2.371 <i>m</i>	2.861	1.377	1.353	91.0

*t*=top, *r*=right, *l*=left

	<i>MP2/aug-cc-pvdz</i>
$\omega_1 a$	3172 <b>2372</b>
$\omega_2 a$	2733 <b>21</b>
$\omega_3 a$	2729 <b>15</b>
$\omega_4 a$	2725 <b>16</b>
$\omega_5 a$	2709 <b>31</b>
$\omega_6 a$	2542 <b>606</b>
$\omega_7 a$	2438 <b>937</b>
$\omega_8 a$	2400 <b>450</b>
$\omega_9 a$	1188 <b>9</b>
$\omega_{10} a$	1186 <b>13</b>
$\omega_{11} a$	1182 <b>7</b>
$\omega_{12} a$	866 <b>28</b>
$\omega_{13} a$	768 <b>36</b>
$\omega_{14} a$	525 <b>8</b>
$\omega_{15} a$	506 <b>9</b>
$\omega_{16} a$	462 <b>8</b>
$\omega_{17} a$	348 <b>1</b>
$\omega_{18} a$	344 <b>6</b>
$\omega_{19} a$	276 <b>1</b>
$\omega_{20} a$	273 <b>16</b>
$\omega_{21} a$	235 <b>8</b>
$\omega_{22} a$	227 <b>9</b>
$\omega_{23} a$	214 <b>27</b>
$\omega_{24} a$	205 <b>9</b>
$\omega_{25} a$	156 <b>&lt;1</b>
$\omega_{26} a$	136 <b>28</b>
$\omega_{27} a$	102 <b>8</b>
$\omega_{28} a$	96 <b>8</b>
$\omega_{29} a$	81 <b>3</b>
$\omega_{30} a$	59 <b>2</b>
$\omega_{31} a$	54 <b>1</b>
$\omega_{32} a$	17 <b>&lt;1</b>
$\omega_{33} a$	13 <b>&lt;1</b>



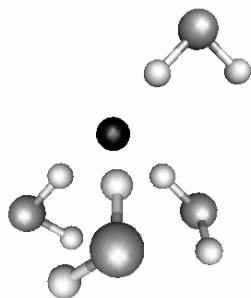
$C_1$  symmetry, minimum

	$r(F-H_b)$	$r(S-H_b)$	$r(S-H_t)$	$\theta(F-H_b-S)$	$\theta(H-S-H)$	$\theta(H_b-F-H_b)$	$zpe$	$E_{MP2}$	$E_{e/BSSE}$	$\Delta E_{e/BSSE}$	$\Delta E_{e/BSSE/Corr}$
<i>pvdz</i>	1.693 <i>tl</i>	1.387	1.351	172.3	91.6	134.0 <i>tl-tr</i>	43.1	-1695.194551	-1695.184940	2.2	1.3
	1.670 <i>tr</i>	1.391	1.350	173.4	91.9	91.1 <i>tr-br</i>					
	1.676 <i>bl</i>	1.390	1.351	172.9	91.7	90.7 <i>br-bl</i>					
	1.630 <i>br</i>	1.399	1.350	175.7	92.4	90.4 <i>bl-tl</i>					

*tl*=top left, *tr*=top right, *bl*=bottom left, *br*=bottom right

	<i>MP2/aug-cc-pvdz</i>
$\omega_1 a$	2757 <b>3</b>
$\omega_2 a$	2755 <b>1</b>
$\omega_3 a$	2753 < <b>1</b>
$\omega_4 a$	2752 < <b>1</b>
$\omega_5 a$	2431 <b>57</b>
$\omega_6 a$	2237 <b>1929</b>
$\omega_7 a$	2205 <b>1949</b>
$\omega_8 a$	2104 <b>1185</b>
$\omega_9 a$	1228 <b>2</b>
$\omega_{10} a$	1221 <b>11</b>
$\omega_{11} a$	1213 <b>12</b>
$\omega_{12} a$	1210 <b>11</b>
$\omega_{13} a$	692 <b>28</b>
$\omega_{14} a$	648 <b>24</b>
$\omega_{15} a$	614 <b>5</b>
$\omega_{16} a$	602 <b>8</b>
$\omega_{17} a$	357 <b>30</b>
$\omega_{18} a$	329 <b>23</b>
$\omega_{19} a$	329 <b>7</b>
$\omega_{20} a$	321 <b>10</b>
$\omega_{21} a$	216 <b>121</b>
$\omega_{22} a$	212 <b>116</b>
$\omega_{23} a$	202 <b>74</b>
$\omega_{24} a$	173 <b>1</b>
$\omega_{25} a$	143 <b>17</b>
$\omega_{26} a$	136 <b>27</b>
$\omega_{27} a$	127 <b>20</b>
$\omega_{28} a$	43 <b>1</b>
$\omega_{29} a$	40 <b>2</b>
$\omega_{30} a$	35 <b>5</b>
$\omega_{31} a$	33 < <b>1</b>
$\omega_{32} a$	18 < <b>1</b>
$\omega_{33} a$	15 <b>1</b>



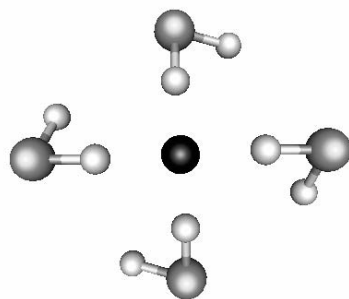


$C_1$  symmetry, minimum

	$r(F-H_b)$	$r(S-H_b)$	$r(S-H_l)$	$\theta(F-H_b-S)$	$\theta(H-S-H)$	$\theta(H_b-F-H_b)$	$zpe$	$E_{MP2}$	$E_e/BSSE$	$\Delta E_e/BSSE$	$\Delta E_e/BSSE/Corr$
<i>pvdz</i>	1.660 <i>t</i>	1.392	1.350	173.5	92.0	90.3 <i>t-r</i>	43.3	-1695.195068	-1695.185210	2.1	1.4
	1.676 <i>r</i>	1.391	1.351	174.2	91.4	89.6 <i>r-m</i>					
	1.675 <i>m</i>	1.390	1.351	171.6	91.5	91.0 <i>m-l</i>					
	1.681 <i>l</i>	1.390	1.351	171.6	91.4	123.0 <i>l-t</i>					

*t*=top, *r*=right, *m*=middle, *l*=left

	<i>MP2/aug-cc-pvdz</i>
$\omega_1 a$	2754 <b>1</b>
$\omega_2 a$	2750 <b>1</b>
$\omega_3 a$	2749 <b>1</b>
$\omega_4 a$	2748 < <b>1</b>
$\omega_5 a$	2434 <b>215</b>
$\omega_6 a$	2203 <b>1395</b>
$\omega_7 a$	2195 <b>1983</b>
$\omega_8 a$	2183 <b>1086</b>
$\omega_9 a$	1223 <b>9</b>
$\omega_{10} a$	1216 <b>11</b>
$\omega_{11} a$	1213 <b>16</b>
$\omega_{12} a$	1207 <b>8</b>
$\omega_{13} a$	654 <b>31</b>
$\omega_{14} a$	636 <b>32</b>
$\omega_{15} a$	627 <b>13</b>
$\omega_{16} a$	617 <b>1</b>
$\omega_{17} a$	341 <b>34</b>
$\omega_{18} a$	336 <b>18</b>
$\omega_{19} a$	326 <b>4</b>
$\omega_{20} a$	325 <b>8</b>
$\omega_{21} a$	254 < <b>1</b>
$\omega_{22} a$	224 <b>164</b>
$\omega_{23} a$	192 <b>100</b>
$\omega_{24} a$	176 <b>12</b>
$\omega_{25} a$	155 <b>11</b>
$\omega_{26} a$	152 <b>59</b>
$\omega_{27} a$	128 <b>4</b>
$\omega_{28} a$	113 <b>11</b>
$\omega_{29} a$	47 <b>1</b>
$\omega_{30} a$	41 <b>1</b>
$\omega_{31} a$	39 <b>1</b>
$\omega_{32} a$	28 <b>1</b>
$\omega_{33} a$	14 < <b>1</b>

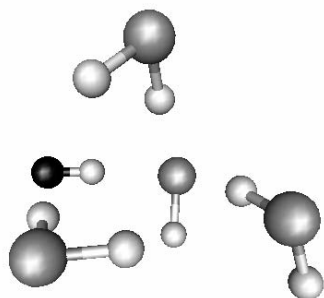


$C_2$  symmetry, minimum

	$r(F-H_b)$	$r(S-H_b)$	$r(S-H_t)$	$\theta(F-H_b-S)$	$\theta(H-S-H)$	$\theta(H_b-F-H_b)$	$zpe$	$E_{MP2}$	$E_{e/BSSE}$	$\Delta E_{e/BSSE}$	$\Delta E_{e/BSSE/Corr}$
<i>pvdz</i>	1.684 <i>t/b</i> 1.680 <i>l/r</i>	1.389 1.390	1.351 1.351	176.6 173.1	91.8 91.9	84.9 <i>t-l/b-r</i> 86.3 <i>l-b/r-t</i>	43.3	-1695.193520	-1695.183815	2.9	2.2

*t*=top, *b*=bottom, *l*=left, *r*=right

	<i>MP2/aug-cc-pvdz</i>
$\omega_1 a$	2753 <1
$\omega_2 a$	2751 <1
$\omega_3 a$	2446 <b>205</b>
$\omega_4 a$	2198 <b>59</b>
$\omega_5 a$	1241 <1
$\omega_6 a$	1203 <b>2</b>
$\omega_7 a$	627 <b>3</b>
$\omega_8 a$	618 <b>7</b>
$\omega_9 a$	342 <b>6</b>
$\omega_{10} a$	332 <b>18</b>
$\omega_{11} a$	222 <b>7</b>
$\omega_{12} a$	199 <b>15</b>
$\omega_{13} a$	112 <b>2</b>
$\omega_{14} a$	82 <b>1</b>
$\omega_{15} a$	46 <1
$\omega_{16} a$	38 <1
$\omega_{17} a$	10 <1
$\omega_{18} b$	2752 <b>1</b>
$\omega_{19} b$	2752 <1
$\omega_{20} b$	2212 <b>1889</b>
$\omega_{21} b$	2202 <b>2368</b>
$\omega_{22} b$	1232 <b>5</b>
$\omega_{23} b$	1210 <b>21</b>
$\omega_{24} b$	637 <b>37</b>
$\omega_{25} b$	597 <b>23</b>
$\omega_{26} b$	353 <b>24</b>
$\omega_{27} b$	324 <b>15</b>
$\omega_{28} b$	197 <b>153</b>
$\omega_{29} b$	187 <b>124</b>
$\omega_{30} b$	170 <b>70</b>
$\omega_{31} b$	154 <b>11</b>
$\omega_{32} b$	47 <b>2</b>
$\omega_{33} b$	44 <b>2</b>



$C_1$  symmetry, minimum

HF-SH<sup>-</sup> unit

	$r(F-H_b)$	$r(S-H_b)$	$r(S-H_d)$	$\theta(F-H_b-S)$	$\theta(H-S-H)$	$zpe$	$E_{MP2}$	$E_{e/BSSE}$	$\Delta E_{e/BSSE}$	$\Delta E_{e/BSSE/Corr}$
<i>pvdz</i>	0.985	1.973	1.354	174.0	88.5	44.2	-1695.195754	-1695.184976	2.2	2.4

SH<sub>2</sub> bound to F and SH<sub>2</sub>

	$r(H...F)$	$r(H...SH_2)$	$r(S-H_F)$	$r(S-H_S)$	$\theta(H-S-H)$
<i>pvdz</i>	2.086	2.734	1.357	1.356	93.0

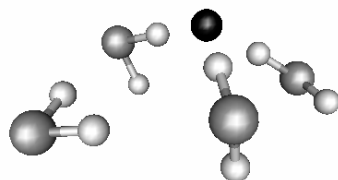
SH<sub>2</sub> bound to S<sup>-</sup> only

	$r(H...S)$	$r(S-H_S)$	$r(S-H_d)$	$\theta(H-S-H)$
<i>pvdz</i>	2.291	1.386	1.351	92.0

SH<sub>2</sub> bound to S<sup>-</sup> and SH<sub>2</sub>

	$r(H...S)$	$r(H...SH_2)$	$r(S-H_S)$	$r(S-H_{SH_2})$	$\theta(H-S-H)$
<i>pvdz</i>	2.418	2.904	1.370	1.352	91.6

	<i>MP2/aug-cc-pvdz</i>
$\omega_1 a$	2826 <b>2016</b>
$\omega_2 a$	2747 <b>6</b>
$\omega_3 a$	2737 <b>16</b>
$\omega_4 a$	2718 <b>24</b>
$\omega_5 a$	2696 <b>24</b>
$\omega_6 a$	2668 <b>314</b>
$\omega_7 a$	2503 <b>577</b>
$\omega_8 a$	2293 <b>1181</b>
$\omega_9 a$	1201 <b>6</b>
$\omega_{10} a$	1198 <b>1</b>
$\omega_{11} a$	1191 <b>2</b>
$\omega_{12} a$	945 <b>38</b>
$\omega_{13} a$	864 <b>45</b>
$\omega_{14} a$	529 <b>7</b>
$\omega_{15} a$	449 <b>1</b>
$\omega_{16} a$	395 <b>5</b>
$\omega_{17} a$	369 <b>20</b>
$\omega_{18} a$	360 <b>22</b>
$\omega_{19} a$	297 <b>3</b>
$\omega_{20} a$	263 <b>19</b>
$\omega_{21} a$	253 <b>5</b>
$\omega_{22} a$	228 <b>27</b>
$\omega_{23} a$	217 <b>5</b>
$\omega_{24} a$	184 <b>5</b>
$\omega_{25} a$	178 <b>6</b>
$\omega_{26} a$	138 <b>37</b>
$\omega_{27} a$	107 <b>3</b>
$\omega_{28} a$	95 <b>10</b>
$\omega_{29} a$	74 <b>1</b>
$\omega_{30} a$	61 <b>1</b>
$\omega_{31} a$	51 <b>1</b>
$\omega_{32} a$	36 <b>1</b>
$\omega_{33} a$	21 <b>1</b>



$C_1$  symmetry, minimum

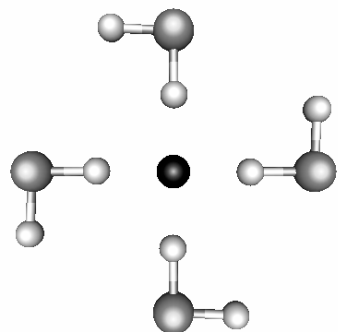
	$r(F-H_b)$	$r(S-H_b)$	$r(S-H_l)$	$\theta(F-H_b-S)$	$\theta(H-S-H)$	$zpe$	$E_{MP2}$	$E_{e/BSSE}$	$\Delta E_{e/BSSE}$	$\Delta E_{e/BSSE/Corr}$
<i>pvdz</i>	1.666 <i>r</i>	1.392	1.350	174.1	91.9	42.7	-1695.191589	-1695.181048	4.7	3.4
	1.501 <i>m</i>	1.430	1.351	177.9	92.8					
	1.510 <i>l</i>	1.426	1.350	179.3	93.0					

*r*=right, *m*=middle, *l*=left

SH<sub>2</sub> bound to two SH<sub>2</sub>'s

	$r(H...SH_2/m)$	$r(H...SH_2/l)$	$r(S-H_{SH_2/m})$	$r(S-H_{SH_2/l})$	$\theta(H-S-H)$
<i>pvdz</i>	2.616	2.606	1.359	1.359	91.6

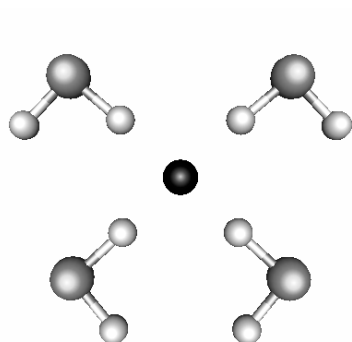
	<i>MP2/aug-cc-pvdz</i>
$\omega_1 a$	2755 <b>1</b>
$\omega_2 a$	2754 <b>3</b>
$\omega_3 a$	2751 <b>3</b>
$\omega_4 a$	2654 <b>228</b>
$\omega_5 a$	2641 <b>241</b>
$\omega_6 a$	2301 <b>694</b>
$\omega_7 a$	1925 <b>1549</b>
$\omega_8 a$	1660 <b>3396</b>
$\omega_9 a$	1238 <b>3</b>
$\omega_{10} a$	1227 <b>2</b>
$\omega_{11} a$	1213 <b>6</b>
$\omega_{12} a$	1198 < <b>1</b>
$\omega_{13} a$	795 <b>26</b>
$\omega_{14} a$	753 <b>7</b>
$\omega_{15} a$	623 <b>15</b>
$\omega_{16} a$	398 <b>6</b>
$\omega_{17} a$	391 <b>24</b>
$\omega_{18} a$	382 <b>6</b>
$\omega_{19} a$	371 < <b>1</b>
$\omega_{20} a$	335 <b>31</b>
$\omega_{21} a$	270 <b>2</b>
$\omega_{22} a$	235 <b>31</b>
$\omega_{23} a$	191 <b>195</b>
$\omega_{24} a$	167 <b>125</b>
$\omega_{25} a$	153 <b>181</b>
$\omega_{26} a$	137 <b>26</b>
$\omega_{27} a$	99 <b>6</b>
$\omega_{28} a$	92 <b>4</b>
$\omega_{29} a$	73 <b>10</b>
$\omega_{30} a$	39 < <b>1</b>
$\omega_{31} a$	25 < <b>1</b>
$\omega_{32} a$	16 < <b>1</b>
$\omega_{33} a$	8 < <b>1</b>



$C_{4h}$  symmetry, 4 imaginary frequencies ( $a_u$ ,  $b_u$ , and  $2e_g$ )

	$r(F-H_b)$	$r(S-H_b)$	$r(S-H_d)$	$\theta(F-H_b-S)$	$\theta(H-S-H)$	$\theta(H_b-F-H_b)$	$zpe$	$E_{MP2}$	$E_{e/BSSE}$	$\Delta E_{e/BSSE}$	$\Delta E_{e/BSSE/Corr}$
<i>pvdz</i>	1.668	1.391	1.350	179.1	92.8	90.0	42.2	-1695.191076	-1695.181994	4.1	2.3

	<i>MP2/aug-cc-pvdz</i>
$\omega_1 a_g$	2757 <b>0</b>
$\omega_2 a_g$	2432 <b>0</b>
$\omega_3 a_g$	1208 <b>0</b>
$\omega_4 a_g$	330 <b>0</b>
$\omega_5 a_g$	152 <b>0</b>
$\omega_6 a_u$	625 <b>15</b>
$\omega_7 a_u$	34 <b>0</b>
$\omega_8 a_u$	145i <b>41</b>
$\omega_9 b_g$	2758 <b>0</b>
$\omega_{10} b_g$	2185 <b>0</b>
$\omega_{11} b_g$	1268 <b>0</b>
$\omega_{12} b_g$	375 <b>0</b>
$\omega_{13} b_g$	92 <b>0</b>
$\omega_{14} b_g$	24 <b>0</b>
$\omega_{15} b_u$	518 <b>0</b>
$\omega_{16} b_u$	102 <b>0</b>
$\omega_{17} b_u$	17i <b>0</b>
$\omega_{18} e_g$	583 <b>0</b>
$\omega_{19} e_g$	75i <b>0</b>
$\omega_{20} e_u$	2758 <b>7 (14)</b>
$\omega_{21} e_u$	2180 <b>2862 (5724)</b>
$\omega_{22} e_u$	1234 <b>3 (6)</b>
$\omega_{23} e_u$	357 <b>73 (146)</b>
$\omega_{24} e_u$	202 <b>230 (460)</b>
$\omega_{25} e_u$	24 <b>1 (2)</b>



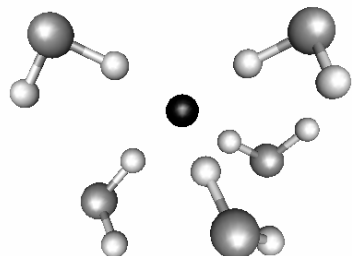
$C_s$  symmetry, 4 imaginary frequencies (all  $a''$ )

	$r(F-H_t)$	$r(S-H_b)$	$r(S-H_t)$	$\theta(F-H_b-S)$	$\theta(H-S-H)$	$\theta(H_b-F-H_b)$	$zpe$	$E_{MP2}$	$E_{e/BSSE}$	$\Delta E_{e/BSSE}$	$\Delta E_{e/BSSE/Corr}$
<i>pvdz</i>	1.703 <i>t</i> 1.644 <i>b</i>	1.386 1.397	1.350 1.349	176.4 178.8	92.5 93.3	92.9 <i>t-t</i> 87.2 <i>t-b</i> 92.7 <i>b-b</i>	42.3	-1695.1905543	-1695.181365	4.5	2.8

*t*=top, *b*=bottom.

	<i>MP2/aug-cc-pvdz</i>
$\omega_1 a'$	2761 <b>9</b>
$\omega_2 a'$	2760 <b>7</b>
$\omega_3 a'$	2756 <b>4</b>
$\omega_4 a'$	2756 <b>1</b>
$\omega_5 a'$	2439 <b>32</b>
$\omega_6 a'$	2260 <b>1515</b>
$\omega_7 a'$	2166 <b>2491</b>
$\omega_8 a'$	2106 <b>1568</b>
$\omega_9 a'$	1269 <b>1</b>
$\omega_{10} a'$	1238 < <b>1</b>
$\omega_{11} a'$	1230 <b>10</b>
$\omega_{12} a'$	1207 < <b>1</b>
$\omega_{13} a'$	390 <b>47</b>
$\omega_{14} a'$	361 <b>39</b>
$\omega_{15} a'$	353 <b>30</b>
$\omega_{16} a'$	328 <b>26</b>
$\omega_{17} a$	206 <b>259</b>
$\omega_{18} a$	193 <b>193</b>
$\omega_{19} a$	149 <b>9</b>
$\omega_{20} a$	89 < <b>1</b>
$\omega_{21} a$	46 < <b>1</b>
$\omega_{22} a$	39 <b>1</b>
$\omega_{23} a$	28 <b>1</b>
$\omega_{24} a''$	636 <b>12</b>
$\omega_{25} a$	592 <b>0</b>
$\omega_{26} a$	567 <b>2</b>
$\omega_{27}$	506 <b>0</b>
$\omega_{28} a''$	100 < <b>1</b>
$\omega_{29} a''$	35 < <b>1</b>
$\omega_{30} a''$	13 <i>i</i> <b>0</b>
$\omega_{31} a''$	37 <i>i</i> <b>0</b>
$\omega_{32} a''$	109 <i>i</i> <b>38</b>
$\omega_{33} a''$	175 <i>i</i> <b>0</b>

## Hexamer Structures: F<sup>-</sup>-(H<sub>2</sub>S)<sub>5</sub>

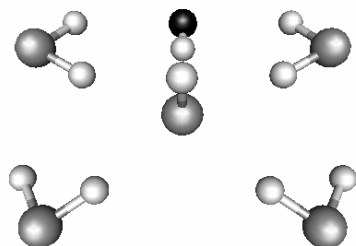


*C*<sub>1</sub> symmetry, minimum

	<i>r</i> (F-H <sub>b</sub> )	<i>r</i> (S-H <sub>b</sub> )	<i>r</i> (S-H <sub>t</sub> )	∠(F-H <sub>b</sub> -S)	∠(H-S-H)	∠(H <sub>b</sub> -F-H <sub>b</sub> )	<i>zpe</i>	<i>E</i> <sub>MP2</sub>	<i>E</i> <sub><i>e</i>/BSSE</sub>	Δ <i>E</i> <sub><i>e</i>/BSSE</sub>	Δ <i>E</i> <sub><i>e</i>/BSSE/Corr</sub>
<i>pvdz</i>	1.732 <i>rb</i>	1.383	1.352	171.5	91.2	88.4 <i>rb-rm</i>	54.4	-2094.065047	-2094.052606	0.0	0.0
	1.790 <i>rm</i>	1.376	1.352	169.6	91.2	86.4 <i>rm-rt</i>					
	1.747 <i>rt</i>	1.380	1.351	170.7	91.4	106.4 <i>rt-lt</i>					
	1.752 <i>lt</i>	1.379	1.351	171.6	91.6	85.4 <i>lt-lb</i>					
	1.752 <i>lb</i>	1.379	1.351	172.3	91.4	87.1 <i>lb-rb</i>					

*rb*=right bottom, *rm*=right middle, *rt*=right top, *lt*=left top, *lb*=left bottom.

	<i>MP2/aug-cc-pvdz</i>
<b>ω<sub>1</sub> a</b>	2751 <b>1</b>
<b>ω<sub>2</sub> a</b>	2749 <b>1</b>
<b>ω<sub>3</sub> a</b>	2747 <b>2</b>
<b>ω<sub>4</sub> a</b>	2744 <b>4</b>
<b>ω<sub>5</sub> a</b>	2742 <b>1</b>
<b>ω<sub>6</sub> a</b>	2544 <b>50</b>
<b>ω<sub>7</sub> a</b>	2396 <b>1091</b>
<b>ω<sub>8</sub> a</b>	2362 <b>658</b>
<b>ω<sub>9</sub> a</b>	2349 <b>1540</b>
<b>ω<sub>10</sub> a</b>	2313 <b>561</b>
<b>ω<sub>11</sub> a</b>	1217 <b>9</b>
<b>ω<sub>12</sub> a</b>	1207 <b>9</b>
<b>ω<sub>13</sub> a</b>	1205 <b>5</b>
<b>ω<sub>14</sub> a</b>	1202 <b>4</b>
<b>ω<sub>15</sub> a</b>	1198 <b>15</b>
<b>ω<sub>16</sub> a</b>	612 <b>29</b>
<b>ω<sub>17</sub> a</b>	576 <b>38</b>
<b>ω<sub>18</sub> a</b>	570 <b>9</b>
<b>ω<sub>19</sub> a</b>	544 <b>11</b>
<b>ω<sub>20</sub> a</b>	528 <b>12</b>
<b>ω<sub>21</sub> a</b>	314 <b>28</b>
<b>ω<sub>22</sub> a</b>	310 <b>33</b>
<b>ω<sub>23</sub> a</b>	294 <b>17</b>
<b>ω<sub>24</sub> a</b>	289 <b>5</b>
<b>ω<sub>25</sub> a</b>	287 <b>7</b>
<b>ω<sub>26</sub> a</b>	283 <b>&lt;1</b>
<b>ω<sub>27</sub> a</b>	221 <b>7</b>
<b>ω<sub>28</sub> a</b>	204 <b>119</b>
<b>ω<sub>29</sub> a</b>	187 <b>24</b>
<b>ω<sub>30</sub> a</b>	186 <b>79</b>
<b>ω<sub>31</sub> a</b>	167 <b>5</b>
<b>ω<sub>32</sub> a</b>	154 <b>45</b>
<b>ω<sub>33</sub> a</b>	135 <b>4</b>
<b>ω<sub>34</sub> a</b>	119 <b>11</b>
<b>ω<sub>35</sub> a</b>	90 <b>&lt;1</b>
<b>ω<sub>36</sub> a</b>	58 <b>1</b>
<b>ω<sub>37</sub> a</b>	50 <b>1</b>
<b>ω<sub>38</sub> a</b>	49 <b>&lt;1</b>
<b>ω<sub>39</sub> a</b>	43 <b>&lt;1</b>
<b>ω<sub>40</sub> a</b>	36 <b>1</b>
<b>ω<sub>41</sub> a</b>	21 <b>1</b>
<b>ω<sub>42</sub> a</b>	11 <b>&lt;1</b>



$C_s$  symmetry, minimum

HF-SH<sup>-</sup> unit

	$r(F-H_b)$	$r(S-H_b)$	$r(S-H_d)$	$\theta(F-H_b-S)$	$\theta(H-S-H)$	$zpe$	$E_{MP2}$	$E_{e/BSSE}$	$\Delta E_{e/BSSE}$	$\Delta E_{e/BSSE/Corr}$
<i>pvdz</i>	0.971	2.031	1.353	178.1	98.8	55.0	-2094.065521	-2094.053442	0.5	0.1

SH<sub>2</sub> units bound to FH..SH<sup>-</sup> core

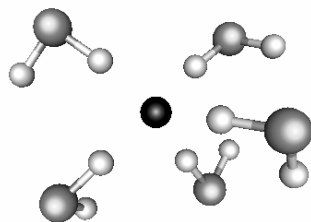
	$r(H...F)$	$r(H...S)$	$r(S-H_F)$	$r(S-H_S)$	$\theta(H-S-H)$
<i>pvdz</i>	2.687	2.408	1.351	1.372	90.9

Bottom SH<sub>2</sub> units bound to SH<sup>-</sup> and SH<sub>2</sub>

	$r(H...SH)$	$r(H...SH_2)$	$r(S-H_S)$	$r(S-H_{SH_2})$	$\theta(H-S-H)$
<i>pvdz</i>	2.422	2.973	1.371	1.351	91.7

	<i>MP2/aug-cc-pvdz</i>
$\omega_1 a'$	3071 <b>1687</b>
$\omega_2 a'$	2752 <b>1</b>
$\omega_3 a'$	2747 <b>4</b>
$\omega_4 a'$	2729 <b>5</b>
$\omega_5 a'$	2525 <b>153</b>
$\omega_6 a'$	2473 <b>654</b>
$\omega_7 a'$	1201 <b>6</b>
$\omega_8 a'$	1183 <b>7</b>
$\omega_9 a'$	870 <b>21</b>
$\omega_{10} a'$	490 <b>6</b>
$\omega_{11} a'$	467 <b>9</b>
$\omega_{12} a'$	322 <b>5</b>
$\omega_{13} a'$	271 <b>16</b>
$\omega_{14} a'$	253 <b>3</b>
$\omega_{15} a'$	228 <b>32</b>
$\omega_{16} a'$	220 <b>13</b>
$\omega_{17} a'$	163 <b>4</b>
$\omega_{18} a'$	104 <b>11</b>
$\omega_{19} a'$	92 <b>1</b>
$\omega_{20} a'$	53 <1
$\omega_{21} a'$	29 <1
$\omega_{22} a'$	26 <b>1</b>
$\omega_{23} a'$	17 <b>1</b>
$\omega_{24} a''$	2752 <b>2</b>
$\omega_{25} a''$	2747 <b>1</b>
$\omega_{26} a''$	2493 <b>1435</b>
$\omega_{27} a''$	2469 <b>911</b>
$\omega_{28} a''$	1199 <1
$\omega_{29} a''$	1183 <b>20</b>
$\omega_{30} a''$	836 <b>66</b>
$\omega_{31} a''$	513 <b>1</b>
$\omega_{32} a''$	461 <b>1</b>
$\omega_{33} a''$	284 <b>1</b>
$\omega_{34} a''$	258 <b>14</b>
$\omega_{35} a''$	244 <b>2</b>
$\omega_{36} a''$	204 <b>9</b>
$\omega_{37} a''$	161 <b>7</b>
$\omega_{38} a''$	150 <b>57</b>
$\omega_{39} a''$	83 <1
$\omega_{40} a''$	60 <b>0</b>
$\omega_{41} a''$	54 <b>1</b>
$\omega_{42} a''$	11 <1

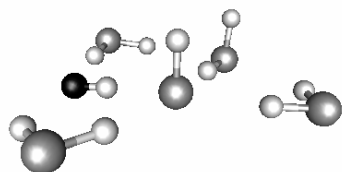




$C_1$  symmetry, minimum

	$r(F-H_b)$	$r(S-H_b)$	$r(S-H_l)$	$\theta(F-H_b-S)$	$\theta(H-S-H)$	$\theta(H_b-F-H_b)$	$zpe$	$E_{MP2}$	$E_{e/BSSE}$	$\Delta E_{e/BSSE}$	$\Delta E_{e/BSSE/Corr}$
<i>pvdz</i>	1.785 <i>tr</i>	1.376	1.352	169.6	91.0	88.1 <i>tr-mr</i>	54.5	-2094.064488	-2094.052168	0.3	0.4
	1.732 <i>mr</i>	1.382	1.351	170.2	91.4	87.8 <i>mr-br</i>					
	1.763 <i>br</i>	1.378	1.352	174.7	91.4	82.2 <i>br-bl</i>					
	1.722 <i>bl</i>	1.383	1.351	174.3	92.1	85.3 <i>bl-tl</i>					
	1.763 <i>tl</i>	1.377	1.351	172.2	91.5	86.6 <i>tl-tr</i>					

	<i>MP2/aug-cc-pvdz</i>
$\omega_1 a$	2755 <1
$\omega_2 a$	2750 1
$\omega_3 a$	2747 2
$\omega_4 a$	2745 2
$\omega_5 a$	2743 2
$\omega_6 a$	2546 47
$\omega_7 a$	2395 911
$\omega_8 a$	2377 1271
$\omega_9 a$	2333 618
$\omega_{10} a$	2311 1195
$\omega_{11} a$	1126 1
$\omega_{12} a$	1217 9
$\omega_{13} a$	1209 15
$\omega_{14} a$	1201 3
$\omega_{15} a$	1199 10
$\omega_{16} a$	614 32
$\omega_{17} a$	580 13
$\omega_{18} a$	570 16
$\omega_{19} a$	559 14
$\omega_{20} a$	536 13
$\omega_{21} a$	318 18
$\omega_{22} a$	317 25
$\omega_{23} a$	305 14
$\omega_{24} a$	302 20
$\omega_{25} a$	284 15
$\omega_{26} a$	277 1
$\omega_{27} a$	211 79
$\omega_{28} a$	203 75
$\omega_{29} a$	188 9
$\omega_{30} a$	178 89
$\omega_{31} a$	164 9
$\omega_{32} a$	154 27
$\omega_{33} a$	126 15
$\omega_{34} a$	110 3
$\omega_{35} a$	84 <1
$\omega_{36} a$	60 1
$\omega_{37} a$	51 1
$\omega_{38} a$	46 <1
$\omega_{39} a$	42 <1
$\omega_{40} a$	34 1
$\omega_{41} a$	20 <1
$\omega_{42} a$	10 <1



$C_1$  symmetry, minimum

HF-SH unit

	$r(F-H_b)$	$r(S-H_b)$	$r(S-H_f)$	$\theta(F-H_b-S)$	$\theta(H-S-H)$	$zpe$	$E_{MP2}$	$E_{e/BSSE}$	$\Delta E_{e/BSSE}$	$\Delta E_{e/BSSE/Corr}$
<i>pvdz</i>	0.983	1.979	1.353	178.2	95.1	54.8	-2094.064185	-2094.052358	0.2	0.6

SH<sub>2</sub> units bound to Fluorine

	$r(H...F)$	$r(H...S)$	$r(S-H_F)$	$r(S-H_S)$	$\theta(H-S-H)$
<i>pvdz</i>	2.567 <i>f</i>	2.449	1.351	1.369	90.8
	2.077 <i>ba</i>	2.696	1.356	1.355	92.3

SH<sub>2</sub> unit bound to SH only

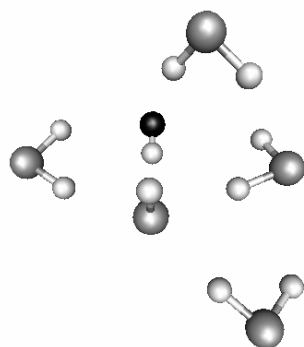
	$r(H...S)$	$r(S-H_S)$	$r(S-H_f)$	$\theta(H-S-H)$
<i>pvdz</i>	2.271	1.391	1.351	92.2

SH<sub>2</sub> unit bound to SH and SH<sub>2</sub>

	$r(H...S)$	$r(H...SH_2)$	$r(S-H_S)$	$r(S-H_{SH_2})$	$\theta(H-S-H)$
<i>pvdz</i>	2.428	2.911	1.369	1.352	91.1

*f*=front, *ba*=back

	<i>MP2/aug-cc-pvdz</i>
$\omega_1 a$	2864 <b>2183</b>
$\omega_2 a$	2756 <b>1</b>
$\omega_3 a$	2754 <b>10</b>
$\omega_4 a$	2737 <b>14</b>
$\omega_5 a$	2728 <b>10</b>
$\omega_6 a$	2700 <b>30</b>
$\omega_7 a$	2684 <b>343</b>
$\omega_8 a$	2525 <b>321</b>
$\omega_9 a$	2513 <b>1231</b>
$\omega_{10} a$	2242 <b>1636</b>
$\omega_{11} a$	1209 <b>2</b>
$\omega_{12} a$	1203 <b>6</b>
$\omega_{13} a$	1184 <b>2</b>
$\omega_{14} a$	1180 <b>32</b>
$\omega_{15} a$	917 <b>25</b>
$\omega_{16} a$	872 <b>72</b>
$\omega_{17} a$	551 <b>10</b>
$\omega_{18} a$	484 <b>3</b>
$\omega_{19} a$	462 <b>6</b>
$\omega_{20} a$	372 <b>10</b>
$\omega_{21} a$	346 <b>13</b>
$\omega_{22} a$	330 <b>1</b>
$\omega_{23} a$	318 <b>8</b>
$\omega_{24} a$	267 <b>4</b>
$\omega_{25} a$	245 <b>13</b>
$\omega_{26} a$	241 <b>23</b>
$\omega_{27} a$	235 <b>8</b>
$\omega_{28} a$	226 <b>3</b>
$\omega_{29} a$	212 <b>21</b>
$\omega_{30} a$	197 <b>9</b>
$\omega_{31} a$	143 <b>63</b>
$\omega_{32} a$	120 <b>16</b>
$\omega_{33} a$	98 <b>6</b>
$\omega_{34} a$	91 <b>1</b>
$\omega_{35} a$	90 <b>1</b>
$\omega_{36} a$	80 <b>3</b>
$\omega_{37} a$	53 < <b>1</b>
$\omega_{38} a$	40 < <b>1</b>
$\omega_{39} a$	24 < <b>1</b>
$\omega_{40} a$	18 <b>1</b>
$\omega_{41} a$	15 < <b>1</b>
$\omega_{42} a$	7 < <b>1</b>



$C_1$  symmetry, minimum

HF-SH<sup>-</sup> unit

	$r(F-H_b)$	$r(S-H_b)$	$r(S-H_l)$	$\theta(F-H_b-S)$	$\theta(H-S-H)$	$zpe$	$E_{MP2}$	$E_{e/BSSE}$	$\Delta E_{e/BSSE}$	$\Delta E_{e/BSSE/Corr}$
<i>pvdz</i>	0.988	1.955	1.354	177.7	94.0	54.8	-2094.064547	-2094.052062	0.3	0.7

SH<sub>2</sub> units bound to FH..SH<sup>-</sup> core

	$r(H...F)$	$r(H...S)$	$r(S-H_F)$	$r(S-H_S)$	$\theta(H-S-H)$
<i>pvdz</i>	3.055 <i>r</i>	2.295	1.351	1.385	91.5
	2.594 <i>l</i>	2.436	1.351	1.370	90.8

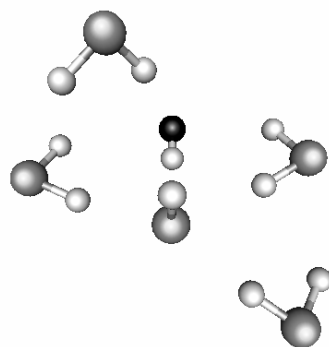
Top SH<sub>2</sub>, bound to F and SH<sub>2</sub>

	$r(H...F)$	$r(H...SH_2)$	$r(S-H_F)$	$r(S-H_{SH_2})$	$\theta(H-S-H)$
<i>pvdz</i>	2.126	2.762	1.355	1.354	91.3

Bottom SH<sub>2</sub> bound to SH<sup>-</sup> and SH<sub>2</sub>

	$r(H...S)$	$r(H...SH_2)$	$r(S-H_S)$	$r(S-H_{SH_2})$	$\theta(H-S-H)$
<i>pvdz</i>	2.397	2.963	1.372	1.351	91.7

	<i>MP2/aug-cc-pvdz</i>
$\omega_1 a$	2776 <b>1313</b>
$\omega_2 a$	2753 <b>135</b>
$\omega_3 a$	2749 <b>14</b>
$\omega_4 a$	2747 <b>29</b>
$\omega_5 a$	2724 <b>8</b>
$\omega_6 a$	2712 <b>54</b>
$\omega_7 a$	2689 <b>563</b>
$\omega_8 a$	2507 <b>332</b>
$\omega_9 a$	2474 <b>1468</b>
$\omega_{10} a$	2308 <b>1087</b>
$\omega_{11} a$	1200 <b>6</b>
$\omega_{12} a$	1198 <b>2</b>
$\omega_{13} a$	1186 <b>22</b>
$\omega_{14} a$	1183 <b>6</b>
$\omega_{15} a$	965 <b>37</b>
$\omega_{16} a$	880 <b>54</b>
$\omega_{17} a$	570 <b>6</b>
$\omega_{18} a$	505 <b>3</b>
$\omega_{19} a$	463 <b>6</b>
$\omega_{20} a$	350 <b>10</b>
$\omega_{21} a$	347 <b>10</b>
$\omega_{22} a$	302 <b>8</b>
$\omega_{23} a$	287 <b>8</b>
$\omega_{24} a$	270 <b>&lt;1</b>
$\omega_{25} a$	260 <b>22</b>
$\omega_{26} a$	250 <b>23</b>
$\omega_{27} a$	229 <b>7</b>
$\omega_{28} a$	223 <b>13</b>
$\omega_{29} a$	197 <b>13</b>
$\omega_{30} a$	190 <b>10</b>
$\omega_{31} a$	153 <b>5</b>
$\omega_{32} a$	150 <b>63</b>
$\omega_{33} a$	114 <b>9</b>
$\omega_{34} a$	95 <b>3</b>
$\omega_{35} a$	92 <b>2</b>
$\omega_{36} a$	79 <b>&lt;1</b>
$\omega_{37} a$	55 <b>&lt;1</b>
$\omega_{38} a$	51 <b>1</b>
$\omega_{39} a$	30 <b>&lt;1</b>
$\omega_{40} a$	22 <b>1</b>
$\omega_{41} a$	15 <b>&lt;1</b>
$\omega_{42} a$	12 <b>&lt;1</b>



$C_1$  symmetry, minimum

HF-SH<sup>-</sup> unit

	$r(F-H_b)$	$r(S-H_b)$	$r(S-H_l)$	$\theta(F-H_b-S)$	$\theta(H-S-H)$	$zpe$	$E_{MP2}$	$E_{e/BSSE}$	$\Delta E_{e/BSSE}$	$\Delta E_{e/BSSE/Corr}$
<i>pvdz</i>	0.988	1.954	1.354	177.6	94.3	54.9	-2094.064435	-2094.051924	0.4	0.9

SH<sub>2</sub> units bound to FH..SH<sup>-</sup> core

	$r(H...F)$	$r(H...S)$	$r(S-H_F)$	$r(S-H_S)$	$\theta(H-S-H)$
<i>pvdz</i>	2.664 <i>r</i>	2.400	1.351 1.351	1.372	90.9
	3.007 <i>l</i>	2.310		1.380	91.5

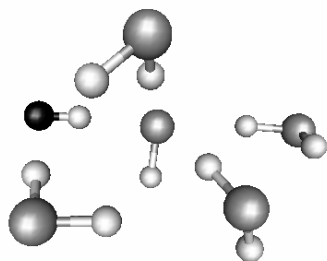
Top SH<sub>2</sub>, bound to F and SH<sub>2</sub>

	$r(H...F)$	$r(H...SH_2)$	$r(S-H_F)$	$r(S-H_{SH_2})$	$\theta(H-S-H)$
<i>pvdz</i>	2.138	2.780	1.355	1.354	91.4

Bottom SH<sub>2</sub> bound to SH<sup>-</sup> and SH<sub>2</sub>

	$r(H...S)$	$r(H...SH_2)$	$r(S-H_S)$	$r(S-H_{SH_2})$	$\theta(H-S-H)$
<i>pvdz</i>	2.403	2.977	1.372	1.351	91.7

	<i>MP2/aug-cc-pvdz</i>
$\omega_1 a$	2773 1271
$\omega_2 a$	2753 21
$\omega_3 a$	2750 88
$\omega_4 a$	2747 16
$\omega_5 a$	2724 8
$\omega_6 a$	2714 68
$\omega_7 a$	2690 580
$\omega_8 a$	2489 1104
$\omega_9 a$	2454 312
$\omega_{10} a$	2367 1568
$\omega_{11} a$	1199 <1
$\omega_{12} a$	1199 8
$\omega_{13} a$	1189 8
$\omega_{14} a$	1182 11
$\omega_{15} a$	968 30
$\omega_{16} a$	883 55
$\omega_{17} a$	559 2
$\omega_{18} a$	494 9
$\omega_{19} a$	476 5
$\omega_{20} a$	347 11
$\omega_{21} a$	345 11
$\omega_{22} a$	291 7
$\omega_{23} a$	280 3
$\omega_{24} a$	271 18
$\omega_{25} a$	263 3
$\omega_{26} a$	257 30
$\omega_{27} a$	247 8
$\omega_{28} a$	223 11
$\omega_{29} a$	211 6
$\omega_{30} a$	163 19
$\omega_{31} a$	161 5
$\omega_{32} a$	148 63
$\omega_{33} a$	110 5
$\omega_{34} a$	94 5
$\omega_{35} a$	94 <1
$\omega_{36} a$	72 1
$\omega_{37} a$	57 <1
$\omega_{38} a$	53 <1
$\omega_{39} a$	32 <1
$\omega_{40} a$	22 1
$\omega_{41} a$	16 <1
$\omega_{42} a$	11 <1



$C_1$  symmetry, minimum

HF-SH<sup>-</sup> unit

	$r(F-H_b)$	$r(S-H_b)$	$r(S-H_f)$	$\theta(F-H_b-S)$	$\theta(H-S-H)$	$zpe$	$E_{MP2}$	$E_{e/BSSE}$	$\Delta E_{e/BSSE}$	$\Delta E_{e/BSSE/Corr}$
<i>pvdz</i>	0.977	2.000	1.354	174.0	91.1	55.1	-2094.064374	-2094.051229	0.9	1.6

Top SH<sub>2</sub>, bound to SH<sup>-</sup> and SH<sub>2</sub>

	$r(H...S)$	$r(H...SH_2)$	$r(S-H_{SH})$	$r(S-H_{SH_2})$	$\theta(H-S-H)$
<i>pvdz</i>	2.458	2.881	1.366	1.352	91.6

Front SH<sub>2</sub>, bound to F and SH<sub>2</sub>

	$r(H...F)$	$r(H...SH_2)$	$r(S-H_F)$	$r(S-H_{SH_2})$	$\theta(H-S-H)$
<i>pvdz</i>	2.098	2.742	1.357	1.355	93.0

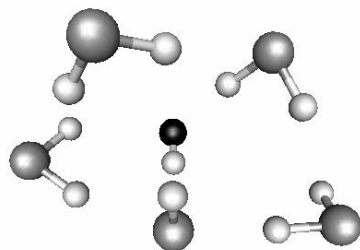
Front SH<sub>2</sub> bound to SH<sup>-</sup>

	$r(H...S)$	$r(S-H_s)$	$r(S-H_f)$	$\theta(H-S-H)$
<i>pvdz</i>	2.304	1.385	1.352	91.9

Right SH<sub>2</sub> bound to SH<sup>-</sup>

	$r(H...S)$	$r(S-H_s)$	$r(S-H_f)$	$\theta(H-S-H)$
<i>pvdz</i>	2.407	1.371	1.352	91.2

	<i>MP2/aug-cc-pvdz</i>
$\omega_1 a$	2965 <b>2258</b>
$\omega_2 a$	2743 <b>4</b>
$\omega_3 a$	2738 <b>10</b>
$\omega_4 a$	2733 <b>22</b>
$\omega_5 a$	2721 <b>13</b>
$\omega_6 a$	2704 <b>42</b>
$\omega_7 a$	2681 <b>169</b>
$\omega_8 a$	2562 <b>383</b>
$\omega_9 a$	2496 <b>922</b>
$\omega_{10} a$	2312 <b>867</b>
$\omega_{11} a$	1201 <b>7</b>
$\omega_{12} a$	1199 <b>1</b>
$\omega_{13} a$	1190 <b>2</b>
$\omega_{14} a$	1183 <b>12</b>
$\omega_{15} a$	905 <b>46</b>
$\omega_{16} a$	827 <b>58</b>
$\omega_{17} a$	538 <b>7</b>
$\omega_{18} a$	490 <b>5</b>
$\omega_{19} a$	421 <b>3</b>
$\omega_{20} a$	388 <b>4</b>
$\omega_{21} a$	364 <b>16</b>
$\omega_{22} a$	353 <b>21</b>
$\omega_{23} a$	306 <b>5</b>
$\omega_{24} a$	263 <b>1</b>
$\omega_{25} a$	249 <b>17</b>
$\omega_{26} a$	238 <b>11</b>
$\omega_{27} a$	232 <b>18</b>
$\omega_{28} a$	223 <b>2</b>
$\omega_{29} a$	221 <b>27</b>
$\omega_{30} a$	189 <b>4</b>
$\omega_{31} a$	159 <b>12</b>
$\omega_{32} a$	137 <b>28</b>
$\omega_{33} a$	111 <b>10</b>
$\omega_{34} a$	99 <b>4</b>
$\omega_{35} a$	91 <b>5</b>
$\omega_{36} a$	77 <b>1</b>
$\omega_{37} a$	65 <b>&lt;1</b>
$\omega_{38} a$	55 <b>1</b>
$\omega_{39} a$	50 <b>2</b>
$\omega_{40} a$	33 <b>&lt;1</b>
$\omega_{41} a$	24 <b>&lt;1</b>
$\omega_{42} a$	8 <b>&lt;1</b>



$C_1$  symmetry, minimum

HF-SH<sup>-</sup> unit

	$r(F-H_b)$	$r(S-H_b)$	$r(S-H_l)$	$\theta(F-H_b-S)$	$\theta(H-S-H)$	$zpe$	$E_{MP2}$	$E_{e/BSSE}$	$\Delta E_{e/BSSE}$	$\Delta E_{e/BSSE/Corr}$
<i>pvdz</i>	0.997	1.927	1.354	177.5	93.9	54.8	-2094.063572	-2094.050227	1.5	1.9

Bottom two SH<sub>2</sub> units bound to FH...SH<sup>-</sup> core

	$r(H...F)$	$r(H...S^{\ominus})$	$r(S-H_F)$	$r(S-H_S)$	$\theta(H-S-H)$
<i>pvdz</i>	4.001 <i>r</i>	2.247	1.351	1.391	92.4
	2.597 <i>l</i>	2.329	1.352	1.379	90.7

Top right SH<sub>2</sub> unit bound to F and SH<sub>2</sub>

	$r(H...F)$	$r(H...SH_2)$	$r(S-H_F)$	$r(S-H_{SH_2})$	$\theta(H-S-H)$
<i>pvdz</i>	2.031	2.720	1.358	1.355	92.1

Top left SH<sub>2</sub> unit bound to two SH<sub>2</sub>'s

	$r(H...SH_2)$	$r(S-H_{SH_2\theta})$	$r(S-H_{SH_2\theta})$	$\theta(H-S-H)$
<i>pvdz</i>	2.707 <i>t</i>	1.355	1.356	93.2
	2.696 <i>l</i>			

*t*=top, *l*=left

	<i>MP2/aug-cc-pvdz</i>
$\omega_1 a$	2754 <b>1</b>
$\omega_2 a$	2749 <b>23</b>
$\omega_3 a$	2719 <b>6</b>
$\omega_4 a$	2705 <b>136</b>
$\omega_5 a$	2701 <b>363</b>
$\omega_6 a$	2685 <b>139</b>
$\omega_7 a$	2680 <b>151</b>
$\omega_8 a$	2570 <b>1716</b>
$\omega_9 a$	2380 <b>632</b>
$\omega_{10} a$	2233 <b>2169</b>
$\omega_{11} a$	1206 <b>1</b>
$\omega_{12} a$	1191 <1
$\omega_{13} a$	1190 <b>9</b>
$\omega_{14} a$	1179 <b>20</b>
$\omega_{15} a$	998 <b>36</b>
$\omega_{16} a$	913 <b>48</b>
$\omega_{17} a$	596 <b>8</b>
$\omega_{18} a$	522 <b>8</b>
$\omega_{19} a$	408 <b>16</b>
$\omega_{20} a$	376 <b>8</b>
$\omega_{21} a$	362 <b>13</b>
$\omega_{22} a$	336 <b>6</b>
$\omega_{23} a$	308 <b>11</b>
$\omega_{24} a$	280 <b>9</b>
$\omega_{25} a$	268 <b>9</b>
$\omega_{26} a$	259 <b>19</b>
$\omega_{27} a$	252 <b>1</b>
$\omega_{28} a$	241 <b>30</b>
$\omega_{29} a$	218 <b>13</b>
$\omega_{30} a$	195 <b>5</b>
$\omega_{31} a$	151 <b>79</b>
$\omega_{32} a$	133 <b>25</b>
$\omega_{33} a$	120 <b>1</b>
$\omega_{34} a$	100 <b>2</b>
$\omega_{35} a$	86 <b>1</b>
$\omega_{36} a$	78 <b>2</b>
$\omega_{37} a$	70 <b>2</b>
$\omega_{38} a$	51 <1
$\omega_{39} a$	44 <1
$\omega_{40} a$	25 <1
$\omega_{41} a$	16 <1
$\omega_{42} a$	14 <1