Supplementary Materials for:

High-resolution FTIR spectroscopy of trisulfane HSSSH: A candidate for detecting parity violation in chiral molecules

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The following content is included as the Supplementary Materials of this publication:

Table S1: Observed rovibrational transitions ($\tilde{\nu}$, in cm^{-1}) for the asymmetric SSH bending fundamental of *trans*-HSSSH. J, K_a and K_c are quantum numbers, $\tilde{\nu}_{obs.}$ = observed wavenumbers and $\tilde{\nu}_{calc.}$ = wavenumbers using the reported spectroscopic parameters (lower states '', upper states ').

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{obs.}$/cm^{-1}	$(\tilde{\nu}_{obs.} - \tilde{\nu}_{calc.})$/$cm^{-1}$
12	4	9	13	4	10	858.78056	0.00002
12	4	9	11	4	8	863.06565	-0.00020
13	5	9	14	5	10	858.60760	0.00000
14	4	11	15	4	12	858.42814	0.00015
13	5	9	12	5	8	863.23226	-0.00008
14	4	11	13	4	10	863.40321	-0.00017
13	5	8	14	5	9	858.60760	0.00002
13	6	8	14	6	9	858.60997	-0.00024
14	5	10	15	5	11	858.43121	-0.00006
13	5	8	12	5	7	863.23226	-0.00011
13	6	8	12	6	7	863.23185	0.00001
14	5	10	13	5	9	863.40040	0.00019
11	9	3	12	9	4	858.96624	-0.00004
12	7	5	13	7	6	858.78827	0.00020
12	8	5	13	8	6	858.78968	-0.00012
13	7	7	14	7	8	858.61266	0.00028
13	6	7	14	6	8	858.60997	-0.00024
14	6	9	15	6	10	858.43422	0.00021
14	5	9	15	5	10	858.43121	-0.00002
15	5	11	16	5	12	858.25484	0.00034
11	9	3	10	9	2	862.89992	-0.00002
12	7	5	11	7	4	863.06514	-0.00003
12	8	5	11	8	4	863.06612	-0.00006
13	6	7	12	6	6	863.23185	0.00001
13	7	7	12	7	6	863.23226	-0.00004
14	6	9	13	6	8	863.39899	-0.00008
14	5	9	13	5	8	863.40040	0.00013
15	5	11	14	5	10	863.56848	0.00049
11	9	2	12	9	3	858.96624	-0.00004
12	8	4	13	8	5	858.78968	-0.00012
13	7	6	14	7	7	858.61266	0.00028
14	7	8	15	7	9	858.43657	0.00031
14	6	8	15	6	9	858.43422	0.00021
15	6	10	16	6	11	858.25719	-0.00019
15	5	10	16	5	11	858.25437	-0.00007
11	9	2	10	9	1	862.89992	-0.00002
12	8	4	11	8	3	863.06612	-0.00006
13	7	6	12	7	5	863.23226	-0.00004
14	7	8	13	7	7	863.39899	-0.00017
14	6	8	13	6	7	863.39899	-0.00008
15	5	10	14	5	9	863.56801	-0.00010
15	6	10	14	6	9	863.56612	0.00001
14	7	7	15	7	8	858.43610	-0.00016

14	8	7	15	8	8	858.43798	-0.00011
14	7	7	13	7	6	863.39899	-0.00017
14	8	7	13	8	6	863.39993	0.00018
14	8	6	15	8	7	858.43798	-0.00011
15	8	8	16	8	9	858.26190	0.00032
17	5	12	18	5	13	857.89933	-0.00018
17	6	12	18	6	13	857.90255	-0.00022
14	8	6	13	8	5	863.39946	-0.00029
15	8	8	14	8	7	863.56612	0.00006
17	5	12	16	5	11	863.90380	0.00006
17	6	12	16	6	11	863.89994	0.00033
13	1	13	14	1	14	858.66789	0.00005
13	1	13	12	1	12	863.06235	-0.00012
10	5	6	11	5	7	859.13432	0.00026
10	4	6	11	4	7	859.13150	0.00016
10	4	6	9	4	5	862.72807	-0.00029
10	5	6	9	5	5	862.72807	0.00004
10	4	7	11	4	8	859.13150	0.00001
10	4	7	9	4	6	862.72807	-0.00013
8	6	3	9	6	4	859.48461	-0.00033
8	5	3	9	5	4	859.48320	0.00025
8	5	3	7	5	2	862.39097	-0.00008
8	6	3	7	6	2	862.39238	0.00003
7	5	2	8	5	3	859.65693	0.00015
8	5	4	9	5	5	859.48273	-0.00022
8	4	4	9	4	5	859.48085	0.00013
7	5	2	6	5	1	862.22242	0.00015
8	4	4	7	4	3	862.39003	-0.00032
8	5	4	7	5	3	862.39097	-0.00008
16	8	9	17	8	10	858.08440	-0.00022
16	7	9	17	7	10	858.08299	0.00028
19	4	15	20	4	16	857.53543	0.00003
16	7	9	15	7	8	863.73186	-0.00021
16	8	9	15	8	8	863.73186	-0.00019
19	4	15	18	4	14	864.26372	0.00029
13	11	2	14	11	3	858.61593	-0.00001
14	11	4	15	11	5	858.43987	-0.00004
14	10	4	15	10	5	858.43987	-0.00021
15	9	6	16	9	7	858.26284	-0.00009
15	10	6	16	10	7	858.26378	0.00017
16	9	8	17	9	9	858.08628	0.00029
16	8	8	17	8	9	858.08440	-0.00022
17	8	10	18	8	11	857.90737	0.00017
19	6	14	20	6	15	857.54590	-0.00044
13	11	2	12	11	1	863.23420	0.00002
14	10	4	13	10	3	863.40040	-0.00034
14	11	4	13	11	3	863.40040	-0.00009

15	9	6	14	9	5	863.56660	0.00008
15	10	6	14	10	5	863.56660	-0.00014
16	8	8	15	8	7	863.73233	0.00028
16	9	8	15	9	7	863.73233	0.00004
17	7	10	16	7	9	863.89806	-0.00005
17	8	10	16	8	9	863.89759	-0.00012
18	6	12	17	6	11	864.06620	0.00008
18	7	12	17	7	11	864.06378	-0.00011
19	6	14	18	6	13	864.23234	-0.00008
15	10	5	16	10	6	858.26378	0.00017
15	11	5	16	11	6	858.26331	-0.00014
16	10	7	17	10	8	858.08675	0.00006
16	9	7	17	9	8	858.08628	0.00029
17	9	9	18	9	10	857.90879	0.00020
17	8	9	18	8	10	857.90737	0.00017
19	6	13	20	6	14	857.54626	-0.00006
20	6	15	21	6	16	857.36734	-0.00007
14	12	3	13	12	2	863.39946	0.00012
14	11	3	13	11	2	863.40040	-0.00009
15	11	5	14	11	4	863.56660	0.00020
15	10	5	14	10	4	863.56660	-0.00014
16	10	7	15	10	6	863.73247	0.00011
16	9	7	15	9	6	863.73247	0.00018
17	8	9	16	8	8	863.89789	0.00018
17	9	9	16	9	8	863.89789	0.00020
18	7	11	17	7	10	864.06378	-0.00011
18	8	11	17	8	10	864.06284	-0.00019
19	6	13	18	6	12	864.23234	-0.00012
19	7	13	18	7	12	864.22951	0.00012
14	13	2	15	13	3	858.43610	0.00002
15	12	4	16	12	5	858.26228	0.00008
15	11	4	16	11	5	858.26331	-0.00014
16	11	6	17	11	7	858.08628	-0.00025
16	10	6	17	10	7	858.08675	0.00006
17	10	8	18	10	9	857.90920	-0.00010
17	9	8	18	9	9	857.90831	-0.00028
18	9	10	19	9	11	857.73082	0.00011
18	8	10	19	8	11	857.72940	0.00010
19	8	12	20	8	13	857.55096	0.00005
20	7	14	21	7	15	857.37017	0.00017
20	6	14	21	6	15	857.36734	-0.00005
21	6	16	22	6	17	857.18796	-0.00004
14	12	2	13	12	1	863.39946	0.00012
15	12	4	14	12	3	863.56519	-0.00001
15	11	4	14	11	3	863.56660	0.00020
16	10	6	15	10	5	863.73247	0.00011
16	11	6	15	11	5	863.73186	-0.00006

17	10	8	16	10	7	863.89759	0.00001
17	9	8	16	9	7	863.89759	-0.00010
18	8	10	17	8	9	864.06284	-0.00019
18	9	10	17	9	9	864.06284	0.00013
19	8	12	18	8	11	864.22810	0.00009
19	7	12	18	7	11	864.22951	0.00012
20	6	14	19	6	13	864.39854	-0.00012
20	7	14	19	7	13	864.39430	-0.00032
21	6	16	20	6	15	864.56458	-0.00003
14	13	1	15	13	2	858.43610	0.00002
15	12	3	16	12	4	858.26228	0.00008
16	11	5	17	11	6	858.08675	0.00022
17	10	7	18	10	8	857.90920	-0.00010
17	11	7	18	11	8	857.90920	0.00006
18	10	9	19	10	10	857.73154	0.00012
18	9	9	19	9	10	857.73082	0.00011
19	9	11	20	9	12	857.55238	0.00005
19	8	11	20	8	12	857.55096	0.00005
20	7	13	21	7	14	857.37017	0.00017
20	8	13	21	8	14	857.37205	0.00004
21	7	15	22	7	16	857.19079	0.00020
21	6	15	22	6	16	857.18796	-0.00001
22	6	17	23	6	18	857.00786	-0.00025
15	12	3	14	12	2	863.56519	-0.00001
16	11	5	15	11	4	863.73186	-0.00006
17	11	7	16	11	6	863.89711	0.00009
17	10	7	16	10	6	863.89759	0.00001
18	9	9	17	9	8	864.06284	0.00013
18	10	9	17	10	8	864.06237	-0.00003
19	8	11	18	8	10	864.22810	0.00009
19	9	11	18	9	10	864.22716	-0.00019
20	8	13	19	8	12	864.39289	0.00024
20	7	13	19	7	12	864.39430	-0.00032
21	6	15	20	6	14	864.56473	0.00000
21	7	15	20	7	14	864.55955	-0.00003
22	5	17	21	5	16	864.74506	-0.00017
22	6	17	21	6	16	864.73046	-0.00003
16	13	4	17	13	5	858.08252	-0.00016
17	11	6	18	11	7	857.90920	0.00006
17	12	6	18	12	7	857.90784	-0.00005
18	10	8	19	10	9	857.73129	-0.00013
18	11	8	19	11	9	857.73129	0.00003
19	9	10	20	9	11	857.55191	-0.00042
19	10	10	20	10	11	857.55285	-0.00019
20	9	12	21	9	13	857.37347	0.00004
20	8	12	21	8	13	857.37174	-0.00027
21	7	14	22	7	15	857.19079	0.00021

21	8	14	22	8	15	857.19262	0.00003
22	7	16	23	7	17	857.01046	-0.00019
22	6	16	23	6	17	857.00811	0.00005
17	11	6	16	11	5	863.89711	0.00009
18	10	8	17	10	7	864.06237	-0.00003
19	9	10	18	9	9	864.22716	-0.00019
19	10	10	18	10	9	864.22669	-0.00011
20	8	12	19	8	11	864.39289	0.00024
21	7	14	20	7	13	864.55955	-0.00004
21	8	14	20	8	13	864.55720	0.00026
22	7	16	21	7	15	864.72434	0.00007
22	6	16	21	6	15	864.73046	-0.00024
16	13	3	17	13	4	858.08252	-0.00016
17	12	5	18	12	6	857.90784	-0.00005
18	11	7	19	11	8	857.73154	0.00028
18	12	7	19	12	8	857.72987	-0.00014
19	10	9	20	10	10	857.55285	-0.00019
19	11	9	20	11	10	857.55285	-0.00003
20	9	11	21	9	12	857.37347	0.00004
20	10	11	21	10	12	857.37394	-0.00020
21	9	13	22	9	14	857.19408	0.00008
21	8	13	22	8	14	857.19262	0.00003
22	7	15	23	7	16	857.01046	-0.00019
22	8	15	23	8	16	857.01282	0.00019
23	7	17	24	7	18	856.83014	-0.00005
24	6	19	25	6	20	856.64699	0.00017
24	5	19	25	5	20	856.64276	-0.00034
16	14	3	15	14	2	863.72432	0.00004
19	10	9	18	10	8	864.22669	-0.00011
19	11	9	18	11	8	864.22575	-0.00017
20	9	11	19	9	10	864.39194	0.00035
20	10	11	19	10	10	864.39053	-0.00024
21	8	13	20	8	12	864.55673	-0.00021
21	9	13	20	9	12	864.55532	-0.00011
22	7	15	21	7	14	864.72434	0.00006
22	8	15	21	8	14	864.72105	0.00019
23	7	17	22	7	16	864.88866	-0.00003
24	5	19	23	5	18	865.08499	0.00011
24	6	19	23	6	18	865.06194	0.00009
18	12	6	19	12	7	857.72987	-0.00014
19	11	8	20	11	9	857.55285	-0.00003
19	12	8	20	12	9	857.55143	-0.00019
20	10	10	21	10	11	857.37394	-0.00020
20	11	10	21	11	11	857.37394	-0.00003
21	9	12	22	9	13	857.19408	0.00008
21	10	12	22	10	13	857.19503	0.00033
22	9	14	23	9	15	857.01423	0.00021

22	8	14	23	8	15	857.01282	0.00019
23	7	16	24	7	17	856.83014	-0.00005
23	8	16	24	8	17	856.83203	-0.00009
24	6	18	25	6	19	856.64699	0.00024
25	6	20	26	6	21	856.46524	-0.00018
25	5	20	26	5	21	856.46196	0.00004
18	13	6	17	13	5	864.05762	-0.00003
19	11	8	18	11	7	864.22575	-0.00017
20	10	10	19	10	9	864.39100	0.00023
21	10	12	20	10	11	864.55438	0.00009
22	8	14	21	8	13	864.72105	0.00019
23	7	16	22	7	15	864.88866	-0.00005
24	7	18	23	7	17	865.05297	0.00013
25	5	20	24	5	19	865.25579	-0.00022
25	6	20	24	6	19	865.22731	-0.00004
20	11	9	21	11	10	857.37394	-0.00003
21	10	11	22	10	12	857.19455	-0.00015
21	11	11	22	11	12	857.19455	0.00003
22	9	13	23	9	14	857.01376	-0.00026
23	9	15	24	9	16	856.83344	-0.00003
23	8	15	24	8	16	856.83203	-0.00009
24	8	17	25	8	18	856.65117	0.00013
25	7	19	26	7	20	856.46761	-0.00001
25	6	19	26	6	20	856.46524	-0.00010
26	5	21	27	5	22	856.28070	0.00030
27	5	23	28	5	24	856.09943	0.00006
18	13	5	17	13	4	864.05762	-0.00003
18	14	5	17	14	4	864.05390	0.00027
21	10	11	20	10	10	864.55438	0.00009
22	10	13	21	10	12	864.71728	-0.00008
24	7	17	23	7	16	865.05297	0.00010
24	8	17	23	8	16	865.04799	0.00038
25	6	19	24	6	18	865.22812	-0.00013
25	7	19	24	7	18	865.21665	-0.00007
26	6	21	25	6	20	865.39241	-0.00030
23	10	14	24	10	15	856.83391	-0.00021
23	9	14	24	9	15	856.83344	-0.00003
24	8	16	25	8	17	856.65117	0.00013
26	7	20	27	7	21	856.28541	-0.00007
26	6	20	27	6	21	856.28352	0.00010
27	6	22	28	6	23	856.10085	-0.00021
27	5	22	28	5	23	856.09896	0.00035
28	5	24	29	5	25	855.91652	-0.00023
28	4	24	29	4	25	855.91534	-0.00007
29	4	26	30	4	27	855.73172	0.00004
21	12	10	20	12	9	864.55131	0.00021
22	10	12	21	10	11	864.71728	-0.00008

22	11	12	21	11	11	864.71587	0.00007
25	7	18	24	7	17	865.21665	-0.00011
26	7	20	25	7	19	865.38019	-0.00014
27	6	22	26	6	21	865.55796	0.00004
29	4	26	28	4	25	865.87184	0.00025
12	3	9	13	3	10	858.77091	0.00003
9	6	3	8	6	2	862.56058	-0.00014
10	6	5	9	6	4	862.72895	0.00011
11	4	7	10	4	6	862.89745	0.00008

Table S2: Calculated ground state combination differences (GSCDs) from observed rovibrational transitions ($\tilde{\nu}$, in cm^{-1}) for the asymmetric SSH bending fundamental of *trans*-HSSSH in Table S1. J, K_a and K_c are quantum numbers, $\tilde{\nu}_{obs.}$ = observed wavenumbers and $\tilde{\nu}_{calc.}$ = wavenumbers using the reported spectroscopic parameters (lower states '', upper states ').

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{GSCD}/cm^{-1}$	$(\tilde{\nu}_{GSCD} - \tilde{\nu}_{calc.})/cm^{-1}$
13	4	10	11	4	8	4.28509	-0.00022
14	5	10	12	5	8	4.62466	-0.00008
15	4	12	13	4	10	4.97507	-0.00032
14	5	9	12	5	7	4.62466	-0.00013
14	6	9	12	6	7	4.62188	0.00025
15	5	11	13	5	9	4.96919	0.00024
12	9	4	10	9	2	3.93368	0.00002
13	7	6	11	7	4	4.27687	-0.00022
13	8	6	11	8	4	4.27644	0.00006
14	6	8	12	6	6	4.62188	0.00025
15	6	10	13	6	8	4.96477	-0.00029
15	5	10	13	5	8	4.96919	0.00015
16	5	12	14	5	10	5.31365	0.00015
12	9	3	10	9	1	3.93368	0.00002
13	8	5	11	8	3	4.27644	0.00006
14	7	7	12	7	5	4.61960	-0.00031
15	7	9	13	7	7	4.96242	-0.00048
15	6	9	13	6	7	4.96477	-0.00029
16	5	11	14	5	9	5.31365	-0.00003
15	8	7	13	8	5	4.96147	-0.00019
16	8	9	14	8	7	5.30422	-0.00025
18	5	13	16	5	11	6.00448	0.00024
18	6	13	16	6	11	5.99739	0.00055
14	1	14	12	1	12	4.39447	0.00010
11	4	7	9	4	5	3.59658	-0.00044
11	5	7	9	5	5	3.59375	-0.00022
11	4	8	9	4	6	3.59658	-0.00013
9	5	4	7	5	2	2.90777	-0.00033
9	6	4	7	6	2	2.90777	0.00036
8	5	3	6	5	1	2.56549	0.00000
9	4	5	7	4	3	2.90918	-0.00044
9	5	5	7	5	3	2.90824	0.00014
17	7	10	15	7	8	5.64887	-0.00049
17	8	10	15	8	8	5.64746	0.00003
20	4	16	18	4	14	6.72829	0.00021
14	11	3	12	11	1	4.61827	0.00003
15	10	5	13	10	3	4.96053	-0.00011
15	11	5	13	11	3	4.96053	-0.00003
16	9	7	14	9	5	5.30376	0.00018
16	10	7	14	10	5	5.30282	-0.00030
17	8	9	15	8	7	5.64793	0.00051
17	9	9	15	9	7	5.64605	-0.00024

18	8	11	16	8	9	5.99021	-0.00029
20	6	15	18	6	13	6.68644	0.00035
16	11	6	14	11	4	5.30329	0.00035
16	10	6	14	10	4	5.30282	-0.00030
17	10	8	15	10	6	5.64571	0.00006
17	9	8	15	9	6	5.64618	-0.00010
18	8	10	16	8	8	5.99052	0.00002
18	9	10	16	9	8	5.98911	0.00002
20	6	14	18	6	12	6.68608	-0.00006
16	12	5	14	12	3	5.30291	-0.00007
16	11	5	14	11	3	5.30329	0.00035
17	10	7	15	10	5	5.64571	0.00006
17	11	7	15	11	5	5.64557	0.00020
18	10	9	16	10	7	5.98838	0.00011
18	9	9	16	9	7	5.98927	0.00018
19	8	11	17	8	9	6.33344	-0.00029
19	9	11	17	9	9	6.33203	0.00003
20	8	13	18	8	11	6.67714	0.00003
21	6	15	19	6	13	7.03119	-0.00009
21	7	15	19	7	13	7.02413	-0.00050
22	6	17	20	6	15	7.37662	0.00000
16	12	4	14	12	2	5.30291	-0.00007
17	11	6	15	11	4	5.64510	-0.00027
18	11	8	16	11	6	5.98791	0.00005
18	10	8	16	10	6	5.98838	0.00011
19	9	10	17	9	8	6.33203	0.00003
19	10	10	17	10	8	6.33083	-0.00014
20	8	12	18	8	10	6.67714	0.00003
20	9	12	18	9	10	6.67478	-0.00024
21	8	14	19	8	12	7.02083	0.00019
21	7	14	19	7	12	7.02413	-0.00050
22	6	16	20	6	14	7.37677	0.00000
22	7	16	20	7	14	7.36877	-0.00023
23	6	18	21	6	16	7.72260	0.00020
18	11	7	16	11	5	5.98791	0.00005
19	10	9	17	10	7	6.33108	0.00012
20	9	11	18	9	9	6.67525	0.00023
20	10	11	18	10	9	6.67384	0.00009
21	8	13	19	8	11	7.02115	0.00051
22	7	15	20	7	13	7.36877	-0.00024
22	8	15	20	8	13	7.36458	0.00023
23	7	17	21	7	15	7.71388	0.00025
23	6	17	21	6	15	7.72235	-0.00030
20	10	10	18	10	8	6.67384	0.00009
20	11	10	18	11	8	6.67290	-0.00013
21	9	12	19	9	10	7.01848	0.00032
21	10	12	19	10	10	7.01660	-0.00003

22	8	14	20	8	12	7.36411	-0.00024
22	9	14	20	9	12	7.36123	-0.00019
23	7	16	21	7	14	7.71388	0.00024
23	8	16	21	8	14	7.70823	-0.00001
24	7	18	22	7	16	8.05851	0.00000
25	5	20	23	5	18	8.44223	0.00039
25	6	20	23	6	18	8.41495	-0.00011
20	11	9	18	11	7	6.67290	-0.00013
21	10	11	19	10	9	7.01707	0.00045
22	10	13	20	10	11	7.35935	-0.00024
23	8	15	21	8	13	7.70823	-0.00001
24	7	17	22	7	15	8.05851	-0.00001
26	5	21	24	5	19	8.79382	-0.00034
26	6	21	24	6	19	8.76207	0.00012
22	10	12	20	10	10	7.35982	0.00024
25	8	18	23	8	16	8.39682	0.00024
26	6	20	24	6	18	8.76288	-0.00007
26	7	20	24	7	18	8.74904	-0.00008
27	7	21	25	7	19	9.09478	-0.00009
28	6	23	26	6	21	9.45711	0.00020
30	4	27	28	4	25	10.14011	0.00016

Table S3: Observed rovibrational transitions ($\tilde{\nu}$, in cm^{-1}) for the fundamental asymmetric SSH bending transition of *cis*-HSSSH. J, K_a and K_c are quantum numbers, $\tilde{\nu}_{obs.}$ = observed wavenumbers and $\tilde{\nu}_{calc.}$ = wavenumbers using the reported spectroscopic parameters (lower states ", upper states ').

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{obs.}/cm^{-1}$	$(\tilde{\nu}_{obs.} - \tilde{\nu}_{calc.})/cm^{-1}$
12	5	7	13	5	8	862.51264	0.00009
12	5	8	13	5	9	862.51264	0.00010
11	5	6	12	5	7	862.67842	-0.00027
11	5	7	12	5	8	862.67842	-0.00026
13	6	7	14	6	8	862.34624	0.00003
13	6	8	14	6	9	862.34624	0.00003
9	3	6	10	3	7	863.01161	-0.00033
9	3	7	10	3	8	863.01161	0.00101
9	4	5	10	4	6	863.01161	0.00060
9	4	6	10	4	7	863.01161	0.00063
9	5	4	10	5	5	863.01161	0.00027
9	5	5	10	5	6	863.01161	0.00027
8	3	5	9	3	6	863.17786	0.00040
8	4	5	9	4	6	863.17786	0.00031
8	5	3	9	5	4	863.17786	-0.00014
8	5	4	9	5	5	863.17786	-0.00014
8	6	2	9	6	3	863.17786	-0.00038
8	6	3	9	6	4	863.17786	-0.00038
10	2	9	11	2	10	862.84325	0.00822
10	6	4	11	6	5	862.84325	-0.00202
10	6	5	11	6	6	862.84325	-0.00202
10	7	3	11	7	4	862.84325	-0.00208
10	7	4	11	7	5	862.84325	-0.00208
10	3	7	11	3	8	862.84531	-0.00236
10	3	8	11	3	9	862.84531	0.00094
10	4	6	11	4	7	862.84531	0.00043
10	4	7	11	4	8	862.84531	0.00055
7	3	4	8	3	5	863.34387	-0.00009
7	3	5	8	3	6	863.34387	-0.00012

Table S4: Calculated (MP2/cc-pVTZ) anharmonic wavenumbers $\tilde{\nu}$ and electric dipole transition moments μ in the double harmonic approximation of *trans*-HSSSH (components according to principal axes).

	fundamental	Γ	$\tilde{\nu}$ / cm-1	μ /Debye	Type
1	s SH stretch	A	2622.498	-0.004	*b*
2	s SSH bend	A	871.64	-0.004	*b*
3	s SS stretch	A	501.975	-0.017	*b*
4	s torsion	A	300.338	0.162	*b*
5	SSS bend	A	206.009	-0.003	*b*
6	as SH stretch	B	2621.73	0.002/-0.001	*a/c*
7	as SSH bend	B	860.564	-0.054/-0.032	*a/c*
8	as SS stretch	B	496.743	0.130/-0.011	*a/c*
9	as torsion	B	324.669	-0.132/0.033	*a/c*

Table S5: Calculated (MP2/cc-pVTZ) anharmonic wavenumbers $\tilde{\nu}$ and electric dipole transition moments μ in the double harmonic approximation of *cis*-HSSSH (components according to principal axes).

	fundamental	Γ	$\tilde{\nu}$ / cm-1	μ /Debye	Type
1	s SH stretch	A`	2616.057	0.007/0.009	*b/c*
2	s SSH bend	A`	874.056	-0.002/-0.039	*b/c*
3	s SS stretch	A`	502.778	0.018/0.002	*b/c*
4	s torsion	A`	325.212	0.131/-0.035	*b/c*
5	SSS bend	A`	206.899	-0.004/-0.009	*b/c*
6	as SH stretch	A``	2619.507	-0.003	*a*
7	as SSH bend	A``	864.807	-0.052	*a*
8	as SS stretch	A``	497.561	-0.135	*a*
9	as torsion	A``	309.145	0.107	*a*