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Supplementary tables for the manuscript:

## **Structural elucidation of 2-fluorothiophenol from Fourier transform microwave spectra and ab initio calculations**

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**Appendix I: Equilibrium Structures from MP2/6-311++G(2d,2p)**

**Appendix II: Assigned Transitions for 2-fluorothiophenol**

## Appendix I: Equilibrium Structures from MP2/6-311++G(2d,2p)

Table 1: Z-matrix structure for *cis*-2-fluorothiophenol

C1						
C2	1	1.393391				
C3	2	1.385588	1	122.7422		
C4	3	1.394415	2	119.0351	1	0.0000
C5	4	1.395775	3	119.6548	2	0.0000
C6	5	1.392892	4	120.2341	3	0.0000
F7	2	1.356154	1	118.8863	6	180.0000
H8	3	1.079820	2	118.9209	1	180.0000
H9	4	1.079795	3	119.7820	2	180.0000
H10	5	1.080112	4	120.2574	3	180.0000
H11	6	1.081288	5	120.0204	4	180.0000
S12	1	1.769470	2	123.1247	3	180.0000
H13	12	1.331296	1	95.7252	2	0.0000

Table 2: Z-matrix structure for *trans*-2-fluorothiophenol

C1						
C2	1	1.393724				
C3	2	1.384799	1	122.8637		
C4	3	1.395099	2	118.8907	1	0.0000
C5	4	1.395290	3	119.6935	2	0.0000
C6	5	1.394132	4	120.3071	3	0.0000
F7	2	1.352699	1	118.1414	6	-180.0000
H8	3	1.079728	2	119.0374	1	180.0000
H9	4	1.079769	3	119.7862	2	180.0000
H10	5	1.080141	4	120.2629	3	-180.0000
H11	6	1.081075	5	119.8192	4	-180.0000
S12	1	1.772407	2	118.1854	3	180.0000

H13      12      1.332261      1      94.4150      2      180.0000

Table 3: Z-matrix structure for thiophenol

C						
C	1	1.398156				
C	2	1.394374	1	120.1787		
C	3	1.395361	2	120.4264	1	0.0000
C	3	2.409578	2	90.1241	1	0.0000
C	5	1.393870	1	29.9484	2	180.0000
H	2	1.081268	1	120.0703	6	-180.0000
H	3	1.080933	2	119.3886	1	-180.0000
H	4	1.080231	3	120.2837	2	-180.0000
H	5	1.080840	6	119.4207	1	-180.0000
H	6	1.081492	5	119.8974	4	-180.0000
S	1	1.777839	6	117.7970	5	180.0000
H	12	1.331982	1	95.9850	6	-180.0000

## Appendix II: Assigned Transitions for 2-fluorothiophenol

Table 1: *cis*-2-fluorothiophenol (parent)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	ν <sub>obs</sub>	ν <sub>calc</sub>	ν <sub>obs-calc</sub>
2	1	2	1	1	1	4577.9708	4577.9723	-0.0015
2	0	2	1	0	1	4985.6710	4985.6700	0.0010
6	2	4	6	2	5	5373.1398	5373.1392	0.0006
4	1	3	4	0	4	5534.9122	5534.9133	-0.0011
2	1	1	1	1	0	5663.6382	5663.6393	-0.0010
2	1	2	1	0	1	5908.1648	5908.1622	0.0026
6	3	3	6	2	4	5920.7999	5920.7999	0.0001
7	3	4	7	2	5	6123.0892	6123.0897	-0.0004
3	0	3	2	1	2	6265.5384	6265.5385	-0.0001
6	2	4	6	1	5	6266.8447	6266.8451	-0.0004
5	3	2	5	2	3	6273.0314	6273.0323	-0.0009
3	2	2	3	1	3	6509.4283	6509.4258	0.0025
2	2	1	2	0	2	6541.5564	6541.5569	-0.0005
3	1	3	2	1	2	6790.8413	6790.8414	-0.0001
11	4	7	11	4	8	6874.8870	6874.8866	0.0004

4	3	1	4	2	2	6898.4889	6898.4877	0.0012
3	2	2	3	0	3	7034.7286	7034.7287	-0.0001
8	3	5	8	2	6	7049.2000	7049.2014	-0.0014
3	0	3	2	0	2	7188.0302	7188.0306	-0.0005
3	3	0	3	2	1	7477.6355	7477.6341	0.0014
9	3	6	9	3	7	7578.2037	7578.2030	0.0007
5	1	4	5	1	5	7598.8609	7598.8607	0.0002
3	2	2	2	2	1	7681.2028	7681.2025	0.0003
4	2	3	4	1	4	7705.5954	7705.5964	-0.0010
5	1	4	5	0	5	7708.1932	7708.1938	-0.0005
4	1	3	3	2	2	7710.5930	7710.5929	0.0001
3	1	3	2	0	2	7713.3341	7713.3336	0.0006
9	4	5	9	3	6	7797.7031	7797.7037	-0.0006
7	2	5	7	2	6	7854.0791	7854.0792	-0.0002
4	2	3	4	0	4	7959.1894	7959.1892	0.0002
3	3	1	3	2	2	8084.1192	8084.1208	-0.0017
10	4	6	10	3	7	8104.2494	8104.2500	-0.0006
3	2	1	2	2	0	8174.3784	8174.3786	-0.0002
8	4	4	8	3	5	8191.2023	8191.2025	-0.0002
7	2	5	7	1	6	8301.3289	8301.3299	-0.0011
3	1	2	2	1	1	8397.5132	8397.5140	-0.0008
4	3	2	4	2	3	8408.0826	8408.0824	0.0002
4	0	4	3	1	3	8685.1055	8685.1055	0.0001
9	3	6	9	2	7	8736.1817	8736.1823	-0.0006
4	1	4	3	1	3	8938.6982	8938.6982	0.0000
5	3	3	5	2	4	8989.8496	8989.8502	-0.0006
7	4	3	7	3	4	9002.2500	9002.2499	0.0001
5	2	4	5	1	5	9177.2699	9177.2695	0.0003
4	0	4	3	0	3	9210.4081	9210.4084	-0.0003
5	2	4	5	0	5	9286.6023	9286.6025	-0.0002
4	1	4	3	0	3	9464.0013	9464.0012	0.0002
2	2	1	1	1	0	9654.2039	9654.2032	0.0007
6	4	2	6	3	3	9871.8338	9871.8348	-0.0010
6	3	4	6	2	5	9873.4212	9873.4208	0.0003
6	1	5	6	1	6	9975.1698	9975.1698	0.0000
6	1	5	6	0	6	10019.0181	10019.0178	0.0003
4	2	3	3	2	2	10134.8688	10134.8688	0.0000
2	2	0	1	1	1	10332.1727	10332.1736	-0.0009
10	3	7	10	3	8	10444.7776	10444.7775	0.0000
4	3	2	3	3	1	10458.8307	10458.8304	0.0003
8	2	6	8	2	7	10494.1302	10494.1294	0.0007

5	4	1	5	3	2	10522.3453	10522.3458	-0.0004
5	3	3	5	1	4	10568.2591	10568.2590	0.0001
4	3	1	3	3	0	10584.0112	10584.0109	0.0002
8	2	6	8	1	7	10698.2633	10698.2630	0.0003
6	3	4	6	1	5	10767.1275	10767.1267	0.0008
4	3	2	4	1	3	10832.3591	10832.3583	0.0008
6	2	5	6	1	6	10868.8761	10868.8756	0.0004
6	2	5	6	0	6	10912.7237	10912.7236	0.0001
5	0	5	4	1	4	10922.3075	10922.3083	-0.0008
5	1	4	4	2	3	10924.9058	10924.9056	0.0002
4	1	3	3	1	2	10984.8454	10984.8454	0.0001
5	1	5	4	1	4	11031.6410	11031.6413	-0.0002
5	4	2	5	3	3	11040.1028	11040.1032	-0.0004
7	3	5	7	2	6	11066.7145	11066.7144	0.0001
4	2	2	3	2	1	11163.1566	11163.1573	-0.0007
6	4	3	6	3	4	11170.4044	11170.4041	0.0003
5	0	5	4	0	4	11175.9008	11175.9010	-0.0003
5	1	5	4	0	4	11285.2333	11285.2340	-0.0007
7	4	4	7	3	5	11498.5852	11498.5850	0.0001
7	3	5	7	1	6	11513.9658	11513.9651	0.0007
3	2	2	2	1	1	11671.7683	11671.7664	0.0019
9	5	4	9	4	5	12001.5754	12001.5755	-0.0001
8	4	5	8	3	6	12096.5291	12096.5291	0.0000
7	1	6	7	1	7	12266.8804	12266.8813	-0.0009
7	1	6	7	0	7	12283.6413	12283.6402	0.0011
5	2	4	4	2	3	12503.3146	12503.3144	0.0002
8	3	6	8	2	7	12540.8936	12540.8932	0.0004
7	2	6	7	1	7	12714.1327	12714.1320	0.0006
7	2	6	7	0	7	12730.8915	12730.8909	0.0006
8	3	6	8	1	7	12745.0255	12745.0268	-0.0013
8	5	3	8	4	4	12950.6928	12950.6920	0.0009
9	4	6	9	3	7	13006.6364	13006.6362	0.0002
6	0	6	5	1	5	13043.5222	13043.5219	0.0003
9	2	7	9	2	8	13081.7239	13081.7240	-0.0001
5	3	3	4	3	2	13085.0818	13085.0822	-0.0005
6	1	6	5	1	5	13087.3697	13087.3699	-0.0002
5	4	2	4	4	1	13100.6405	13100.6403	0.0002
5	4	1	4	4	0	13123.2476	13123.2469	0.0007
6	0	6	5	0	5	13152.8557	13152.8549	0.0008
9	2	7	9	1	8	13169.0577	13169.0579	-0.0002
6	1	6	5	0	5	13196.7029	13196.7029	0.0000

5	1	4	4	1	3	13349.1812	13349.1815	-0.0003
4	2	3	3	1	2	13409.1215	13409.1213	0.0003
5	3	2	4	3	1	13481.3463	13481.3464	-0.0001
7	5	2	7	4	3	13583.7241	13583.7243	-0.0002
6	1	5	5	2	4	13885.2704	13885.2701	0.0002
3	2	1	2	1	2	13928.5802	13928.5798	0.0004
6	5	1	6	4	2	13936.7047	13936.7062	-0.0015
8	5	4	8	4	5	13957.3801	13957.3802	-0.0001
7	5	3	7	4	4	13975.9329	13975.9338	-0.0009
6	5	2	6	4	3	14054.8861	14054.8866	-0.0005
9	5	5	9	4	6	14076.8926	14076.8921	0.0005
5	2	3	4	2	2	14106.8018	14106.8018	0.0000
5	5	0	5	4	1	14113.9065	14113.9069	-0.0004
5	5	1	5	4	2	14139.0714	14139.0707	0.0008
8	4	5	8	2	6	14143.2932	14143.2929	0.0003
9	4	6	9	2	7	14164.6152	14164.6155	-0.0003
10	4	7	10	3	8	14232.6564	14232.6565	-0.0001
9	3	7	9	2	8	14239.7039	14239.7034	0.0005
9	3	7	9	1	8	14327.0375	14327.0373	0.0003
10	5	6	10	4	7	14417.7599	14417.7601	-0.0002
8	1	7	8	1	8	14448.9323	14448.9324	-0.0001
8	1	7	8	0	8	14455.1234	14455.1227	0.0008
8	2	7	8	1	8	14653.0663	14653.0659	0.0003
8	2	7	8	0	8	14659.2563	14659.2562	0.0001
7	4	4	7	2	5	14711.2197	14711.2202	-0.0005
6	2	5	5	2	4	14778.9759	14778.9760	-0.0001
10	4	7	10	2	8	14823.3158	14823.3156	0.0003
3	2	1	2	0	2	14851.0733	14851.0719	0.0014
5	2	4	4	1	3	14927.5901	14927.5903	-0.0003
7	2	5	6	3	4	14948.0112	14948.0102	0.0010
7	0	7	6	1	6	15105.3374	15105.3365	0.0009
7	1	7	6	1	6	15122.0954	15122.0954	-0.0001
7	0	7	6	0	6	15149.1845	15149.1845	0.0000
7	1	7	6	0	6	15165.9435	15165.9434	0.0001
6	1	5	5	1	4	15463.6789	15463.6789	0.0000
10	2	8	10	2	9	15505.6248	15505.6244	0.0003
10	2	8	10	1	9	15541.2878	15541.2883	-0.0006
3	3	1	2	2	0	15630.1867	15630.1868	-0.0001
6	3	4	5	3	3	15662.5464	15662.5466	-0.0002
6	4	3	6	2	4	15670.6852	15670.6857	-0.0005
6	5	2	5	5	1	15708.6632	15708.6634	-0.0002

6	5	1	5	5	0	15712.0831	15712.0826	0.0005
3	3	0	2	2	1	15787.1490	15787.1492	-0.0001
6	4	3	5	4	2	15792.8475	15792.8475	0.0000
6	4	2	5	4	1	15889.2829	15889.2833	-0.0004
11	4	8	11	2	9	16019.5250	16019.5249	0.0002
10	3	8	10	2	9	16096.2843	16096.2835	0.0008
10	3	8	10	1	9	16131.9476	16131.9475	0.0002
6	2	5	5	1	4	16357.3854	16357.3848	0.0007
7	1	6	6	2	5	16520.1009	16520.1011	-0.0002
6	3	3	5	3	2	16539.7936	16539.7943	-0.0006
9	1	8	9	1	9	16554.6184	16554.6181	0.0004
9	6	3	9	5	4	16636.6308	16636.6301	0.0007
9	2	8	9	1	9	16641.9519	16641.9520	-0.0001
9	2	8	9	0	9	16644.1810	16644.1808	0.0002
5	4	2	5	2	3	16769.8656	16769.8650	0.0007
10	6	5	10	5	6	16783.3766	16783.3771	-0.0005
6	2	4	5	2	3	16892.0267	16892.0267	0.0000
9	6	4	9	5	5	16914.0031	16914.0030	0.0001
7	2	6	6	2	5	16967.3513	16967.3518	-0.0005
8	6	2	8	5	3	16977.2996	16977.2997	-0.0002
8	6	3	8	5	4	17064.2858	17064.2841	0.0018
8	0	8	7	1	7	17140.3936	17140.3932	0.0003
8	1	8	7	1	7	17146.5840	17146.5835	0.0005
8	0	8	7	0	7	17157.1526	17157.1521	0.0005
8	1	8	7	0	7	17163.3434	17163.3424	0.0009
7	6	1	7	5	2	17174.4541	17174.4535	0.0007
7	6	2	7	5	3	17195.8602	17195.8598	0.0004
7	1	6	6	1	5	17413.8081	17413.8069	0.0012
11	2	9	11	2	10	17771.4690	17771.4684	0.0006
7	2	6	6	1	5	17861.0581	17861.0576	0.0005
4	3	2	3	2	1	17914.6387	17914.6386	0.0001
7	3	5	6	3	4	18160.6451	18160.6454	-0.0002
10	5	6	10	3	7	18205.6383	18205.6390	-0.0007
4	2	2	3	1	3	18300.8961	18300.8957	0.0004
7	6	2	6	6	1	18311.9606	18311.9604	0.0001
7	6	1	6	6	0	18312.4252	18312.4247	0.0005
7	5	3	6	5	2	18409.8734	18409.8734	0.0000
7	5	2	6	5	1	18428.0149	18428.0149	0.0001
7	4	4	6	4	3	18488.8260	18488.8263	-0.0003
8	2	6	7	3	5	18512.9325	18512.9325	0.0000
10	1	9	10	1	10	18618.4523	18618.4523	0.0001

10	1	9	10	0	10	18619.2377	18619.2390	-0.0012
10	2	9	10	1	10	18654.1168	18654.1162	0.0006
10	2	9	10	0	10	18654.9028	18654.9029	0.0000
4	3	1	3	2	2	18689.9556	18689.9576	-0.0020
7	4	3	6	4	2	18780.9963	18780.9968	-0.0005
4	2	2	3	0	3	18826.1980	18826.1986	-0.0007
8	1	7	7	2	6	18881.3844	18881.3839	0.0005
8	2	7	7	2	6	19085.5168	19085.5174	-0.0007
9	0	9	8	1	8	19164.3956	19164.3956	0.0000
9	1	9	8	1	8	19166.6248	19166.6244	0.0004
9	0	9	8	0	8	19170.5867	19170.5859	0.0008
9	1	9	8	0	8	19172.8144	19172.8147	-0.0003
8	1	7	7	1	6	19328.6351	19328.6346	0.0005
7	2	5	6	2	4	19448.2918	19448.2918	0.0000
9	5	5	9	3	6	19505.3256	19505.3253	0.0003
8	2	7	7	1	6	19532.7683	19532.7681	0.0002
7	3	4	6	3	3	19650.5815	19650.5817	-0.0002
5	3	3	4	2	2	19836.5624	19836.5636	-0.0012
12	2	10	12	2	11	19931.5466	19931.5474	-0.0009
8	3	6	7	3	5	20559.6960	20559.6963	-0.0003
11	1	10	11	1	11	20661.4823	20661.4830	-0.0007
11	2	10	11	0	11	20675.8167	20675.8163	0.0003
8	6	3	7	6	2	21007.5102	21007.5110	-0.0008
8	6	2	7	6	1	21010.4441	21010.4459	-0.0018
9	1	8	8	2	7	21068.1766	21068.1766	0.0000
8	5	4	7	5	3	21139.0874	21139.0867	0.0006
9	2	8	8	2	7	21155.5097	21155.5105	-0.0008
8	4	5	7	4	4	21157.6396	21157.6403	-0.0007
10	0	10	9	1	9	21184.1218	21184.1221	-0.0003
10	1	10	9	1	9	21184.9089	21184.9088	0.0002
10	0	10	9	0	9	21186.3517	21186.3509	0.0008
10	1	10	9	0	9	21187.1381	21187.1376	0.0005
8	5	3	7	5	2	21207.6011	21207.5996	0.0015
9	1	8	8	1	7	21272.3112	21272.3101	0.0011
9	2	8	8	1	7	21359.6450	21359.6440	0.0010
6	3	4	5	2	3	21392.3073	21392.3083	-0.0010
4	4	1	3	3	0	21461.5491	21461.5497	-0.0006
4	4	0	3	3	1	21486.2798	21486.2821	-0.0023
9	2	7	8	3	6	21696.3407	21696.3413	-0.0006
8	2	6	7	2	5	21725.5689	21725.5676	0.0013
8	4	4	7	4	3	21840.6319	21840.6319	0.0000



4	3	1	3	1	2	21964.2135	21964.2101	0.0034
5	3	2	4	2	3	22036.4336	22036.4352	-0.0016
8	3	5	7	3	4	22651.6785	22651.6794	-0.0009
7	3	5	6	2	4	22660.9264	22660.9270	-0.0005
9	3	7	8	3	6	22854.3201	22854.3206	-0.0005
10	1	9	9	2	8	23161.4073	23161.4090	-0.0017
10	2	9	9	2	8	23197.0726	23197.0730	-0.0003
11	1	11	10	1	10	23202.5609	23202.5613	-0.0004
11	0	11	10	0	10	23203.0738	23203.0747	-0.0009
10	1	9	9	1	8	23248.7439	23248.7430	0.0009
10	2	9	9	1	8	23284.4068	23284.4069	-0.0001
9	8	2	8	8	1	23519.9802	23519.9778	0.0025
9	7	3	8	7	2	23604.5949	23604.5926	0.0023
9	7	2	8	7	1	23605.0197	23605.0219	-0.0022
5	2	3	4	0	4	23722.5923	23722.5921	0.0002
9	6	4	8	6	3	23733.6567	23733.6586	-0.0018
9	2	7	8	2	6	23743.1048	23743.1050	-0.0002
9	6	3	8	6	2	23746.8011	23746.8011	0.0000
9	4	6	8	4	5	23764.4275	23764.4277	-0.0002
8	3	6	7	2	5	23772.3314	23772.3314	0.0000
9	5	5	8	5	4	23883.9401	23883.9396	0.0004
5	4	2	4	3	1	23978.1783	23978.1791	-0.0008
9	5	4	8	5	3	24087.4703	24087.4707	-0.0004
5	4	1	4	3	2	24150.6965	24150.6986	-0.0021
5	3	2	4	1	3	24460.7127	24460.7111	0.0016
9	4	5	8	4	4	25036.5857	25036.5872	-0.0016
10	3	8	9	3	7	25053.6541	25053.6531	0.0010
12	1	12	11	1	11	25220.0142	25220.0145	-0.0003
12	0	12	11	0	11	25220.1941	25220.1936	0.0006
11	2	10	10	2	9	25223.9868	25223.9881	-0.0014
11	1	10	10	1	9	25245.5925	25245.5920	0.0005
9	3	6	8	3	5	25430.0874	25430.0860	0.0014
10	2	8	9	2	7	25620.9732	25620.9734	-0.0002

Table 2: *cis*-2-fluorothiophenol ( $^{13}\text{C}1$ )

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	$\nu_{\text{obs}}$	$\nu_{\text{calc}}$	$\nu_{\text{obs-calc}}$
3	1	3	2	1	2	6787.4782	6787.4784	-0.0001
3	0	3	2	0	2	7184.3390	7184.3384	0.0006

3	1	2	2	1	1	8393.7910	8393.7913	-0.0004
4	1	4	3	1	3	8934.1782	8934.1793	-0.0011
4	0	4	3	0	3	9205.5155	9205.5156	-0.0001
4	2	3	3	2	2	10130.1520	10130.1525	-0.0005
4	1	3	3	1	2	10979.7308	10979.7312	-0.0004
5	1	5	4	1	4	11025.9769	11025.9774	-0.0005
5	0	5	4	0	4	11169.9546	11169.9538	0.0008
5	2	4	4	2	3	12497.3379	12497.3384	-0.0005
5	3	3	4	3	2	13079.3034	13079.3035	0.0000
6	1	6	5	1	5	13080.5868	13080.5865	0.0003
6	0	6	5	0	5	13145.9067	13145.9061	0.0006
5	1	4	4	1	3	13342.5425	13342.5422	0.0003
5	3	2	4	3	1	13475.9918	13475.9909	0.0010
5	2	3	4	2	2	14100.9055	14100.9050	0.0005
6	1	5	5	1	4	15455.5253	15455.5255	-0.0002
6	3	4	5	3	3	15655.4951	15655.4945	0.0006
6	4	3	5	4	2	15786.0447	15786.0446	0.0001
6	4	2	5	4	1	15882.6670	15882.6678	-0.0008
6	3	3	5	3	2	16533.4424	16533.4419	0.0005
6	2	4	5	2	3	16884.5428	16884.5438	-0.0010
7	2	6	6	2	5	16958.8196	16958.8196	0.0000
8	1	8	7	1	7	17137.6314	17137.6320	-0.0006
8	0	8	7	0	7	17148.1630	17148.1628	0.0002
7	1	6	6	1	5	17404.3987	17404.3981	0.0007
7	3	5	6	3	4	18152.2465	18152.2468	-0.0003

Table 3: *cis*-2-fluorothiophenol ( $^{13}\text{C}2$ )

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	ν <sub>obs</sub>	ν <sub>calc</sub>	ν <sub>obs-calc</sub>
3	1	3	2	1	2	6782.4502	6782.4515	-0.0013
3	1	2	2	1	1	8392.8982	8392.8991	-0.0010
4	1	4	3	1	3	8926.4442	8926.4431	0.0011
4	0	4	3	0	3	9194.7058	9194.7062	-0.0005
4	1	3	3	1	2	10975.5847	10975.5845	0.0002
5	1	5	4	1	4	11015.3791	11015.3779	0.0012
5	0	5	4	0	4	11156.7143	11156.7145	-0.0002
5	2	4	4	2	3	12490.7270	12490.7273	-0.0004
6	1	6	5	1	5	13067.2380	13067.2386	-0.0006
5	3	3	4	3	2	13078.1608	13078.1605	0.0003

6	0	6	5	0	5	13130.9263	13130.9264	-0.0002
5	1	4	4	1	3	13332.3475	13332.3472	0.0002
5	3	2	4	3	1	13482.0915	13482.0906	0.0009
5	2	3	4	2	2	14103.6819	14103.6821	-0.0002
6	1	5	5	1	4	15438.1353	15438.1355	-0.0001
6	3	4	5	3	3	15652.4749	15652.4742	0.0007
6	4	3	5	4	2	15786.7608	15786.7613	-0.0006
6	4	2	5	4	1	15886.1899	15886.1897	0.0002
6	3	3	5	3	2	16543.5194	16543.5201	-0.0006
6	2	4	5	2	3	16882.7401	16882.7396	0.0005
7	2	6	6	2	5	16944.7219	16944.7219	-0.0001
8	1	8	7	1	7	17119.3739	17119.3718	0.0020
8	0	8	7	0	7	17129.5080	17129.5099	-0.0019
7	1	6	6	1	5	17382.1116	17382.1114	0.0002
7	3	5	6	3	4	18146.0405	18146.0410	-0.0005

Table 4: *cis*-2-fluorothiophenol ( $^{13}\text{C}3$ )

$J'$	$K_a'$	$K_c'$	$J''$	$K_a''$	$K_c''$	$\nu_{\text{obs}}$	$\nu_{\text{calc}}$	$\nu_{\text{obs-calc}}$
3	1	3	2	1	2	6741.1730	6741.1735	-0.0005
3	1	2	2	1	1	8333.6829	8333.6835	-0.0006
4	1	4	3	1	3	8873.8265	8873.8260	0.0005
4	0	4	3	0	3	9144.8503	9144.8498	0.0005
5	1	5	4	1	4	10952.0564	10952.0562	0.0002
5	0	5	4	0	4	11096.4163	11096.4177	-0.0014
5	2	4	4	2	3	12410.6634	12410.6633	0.0001
6	1	6	5	1	5	12993.3063	12993.3063	0.0000
6	0	6	5	0	5	13059.0408	13059.0404	0.0004
5	1	4	4	1	3	13251.6541	13251.6536	0.0006
5	3	2	4	3	1	13375.5067	13375.5085	-0.0018
5	2	3	4	2	2	13997.6270	13997.6260	0.0009
6	2	5	5	2	4	14670.5262	14670.5261	0.0001
6	1	5	5	1	4	15353.2393	15353.2386	0.0007
6	3	4	5	3	3	15544.1092	15544.1078	0.0013
6	4	3	5	4	2	15671.7441	15671.7433	0.0008
6	4	2	5	4	1	15766.1979	15766.1981	-0.0003
6	3	3	5	3	2	16408.7482	16408.7484	-0.0003
6	2	4	5	2	3	16763.5938	16763.5938	-0.0001
7	2	6	6	2	5	16843.9380	16843.9375	0.0005

8	1	8	7	1	7	17023.6988	17023.6987	0.0001
8	0	8	7	0	7	17034.3692	17034.3690	0.0001
7	1	6	6	1	5	17290.6996	17290.7012	-0.0017
7	3	5	6	3	4	18024.5277	18024.5281	-0.0004

Table 5: *cis*-2-fluorothiophenol ( $^{13}\text{C}4$ )

$J'$	$K_a'$	$K_c'$	$J''$	$K_a''$	$K_c''$	$\nu_{\text{obs}}$	$\nu_{\text{calc}}$	$\nu_{\text{obs-calc}}$
3	1	3	2	1	2	6703.2450	6703.2438	0.0013
3	0	3	2	0	2	7102.0475	7102.0464	0.0011
3	1	2	2	1	1	8265.5852	8265.5860	-0.0008
4	1	4	3	1	3	8828.2788	8828.2792	-0.0004
4	0	4	3	0	3	9109.1594	9109.1598	-0.0004
5	1	5	4	1	4	10900.0279	10900.0287	-0.0009
5	0	5	4	0	4	11053.9363	11053.9376	-0.0013
5	2	4	4	2	3	12330.1098	12330.1101	-0.0003
6	1	6	5	1	5	12934.7204	12934.7205	-0.0001
6	0	6	5	0	5	13006.7293	13006.7288	0.0005
5	1	4	4	1	3	13177.0908	13177.0895	0.0013
5	2	3	4	2	2	13865.8736	13865.8749	-0.0012
6	2	5	5	2	4	14584.5160	14584.5143	0.0017
6	1	5	5	1	4	15289.2501	15289.2498	0.0003
6	3	4	5	3	3	15422.4685	15422.4679	0.0006
6	4	3	5	4	2	15534.9232	15534.9231	0.0001
6	4	2	5	4	1	15618.3011	15618.3013	-0.0002
6	3	3	5	3	2	16228.8657	16228.8653	0.0004
7	2	6	6	2	5	16754.7534	16754.7539	-0.0005
8	1	8	7	1	7	16950.1681	16950.1680	0.0001
8	0	8	7	0	7	16962.4643	16962.4641	0.0002
7	1	6	6	1	5	17230.6075	17230.6081	-0.0007
7	3	5	6	3	4	17893.7846	17893.7850	-0.0005

Table 6: *cis*-2-fluorothiophenol ( $^{13}\text{C}5$ )

$J'$	$K_a'$	$K_c'$	$J''$	$K_a''$	$K_c''$	$\nu_{\text{obs}}$	$\nu_{\text{calc}}$	$\nu_{\text{obs-calc}}$
6	0	6	5	0	5	13018.6333	13018.6332	0.0001
6	1	6	5	1	5	12953.7944	12953.7946	-0.0002

5	0	5	4	0	4	11061.8618	11061.8619	-0.0001
4	1	4	3	1	3	8847.4492	8847.4486	0.0006
4	0	4	3	0	3	9116.4258	9116.4254	0.0004
5	1	5	4	1	4	10919.0392	10919.0394	-0.0003
5	2	4	4	2	3	12375.6286	12375.6293	-0.0007
4	1	3	3	1	2	10872.6504	10872.6503	0.0001
4	2	3	3	2	2	10031.3507	10031.3504	0.0004
6	2	4	5	2	3	16719.4391	16719.4393	-0.0002
8	1	8	7	1	7	16971.5874	16971.5875	0.0000
8	0	8	7	0	7	16982.0537	16982.0536	0.0001
3	1	2	2	1	1	8311.7145	8311.7152	-0.0008
3	1	3	2	1	2	6721.5080	6721.5070	0.0010
3	0	3	2	0	2	7114.6633	7114.6651	-0.0018
5	1	4	4	1	3	13212.9057	13212.9055	0.0003
5	2	3	4	2	2	13962.6141	13962.6137	0.0004
6	2	5	5	2	4	14628.0815	14628.0823	-0.0008
6	1	5	5	1	4	15305.8902	15305.8897	0.0006
6	3	4	5	3	3	15502.5343	15502.5336	0.0007
6	4	3	5	4	2	15631.4562	15631.4552	0.0011
6	4	2	5	4	1	15726.8672	15726.8687	-0.0015
6	3	3	5	3	2	16370.6456	16370.6457	-0.0001
7	2	6	6	2	5	16794.1460	16794.1461	-0.0001
7	3	5	6	3	4	17975.1470	17975.1471	-0.0001
5	3	2	4	3	1	13343.5035	13343.5029	0.0006

Table 7: *cis*-2-fluorothiophenol ( $^{13}\text{C}6$ )

$J'$	$K_a'$	$K_c'$	$J''$	$K_a''$	$K_c''$	$\nu_{\text{obs}}$	$\nu_{\text{calc}}$	$\nu_{\text{obs-calc}}$
3	1	3	2	1	2	6765.1810	6765.1816	-0.0006
3	1	2	2	1	1	8382.2771	8382.2778	-0.0007
4	1	4	3	1	3	8901.4330	8901.4327	0.0003
4	0	4	3	0	3	9163.1922	9163.1923	-0.0001
5	1	5	4	1	4	10982.3884	10982.3883	0.0001
5	0	5	4	0	4	11118.3113	11118.3116	-0.0003
4	2	2	3	2	1	11160.2574	11160.2573	0.0001
5	2	4	4	2	3	12464.2098	12464.2101	-0.0003
6	1	6	5	1	5	13026.5570	13026.5565	0.0005
5	3	3	4	3	2	13062.1914	13062.1914	-0.0001
6	0	6	5	0	5	13086.9629	13086.9632	-0.0003

5	1	4	4	1	3	13297.4289	13297.4292	-0.0003
5	3	2	4	3	1	13480.6707	13480.6699	0.0008
5	2	3	4	2	2	14094.3839	14094.3841	-0.0002
6	1	5	5	1	4	15386.4876	15386.4859	0.0018
6	3	4	5	3	3	15629.9267	15629.9252	0.0014
6	4	3	5	4	2	15771.8254	15771.8254	0.0001
6	4	2	5	4	1	15877.0603	15877.0611	-0.0008
6	3	3	5	3	2	16546.8283	16546.8286	-0.0003
6	2	4	5	2	3	16861.0181	16861.0184	-0.0003
7	2	6	6	2	5	16898.3243	16898.3249	-0.0006
8	1	8	7	1	7	17064.5514	17064.5504	0.0011
8	0	8	7	0	7	17073.9193	17073.9202	-0.0009
7	1	6	6	1	5	17318.8036	17318.8046	-0.0010
7	3	5	6	3	4	18114.3201	18114.3200	0.0001

Table 8: *cis*-2-fluorothiophenol ( $^{34}\text{S}$ )

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	$\nu_{\text{obs}}$	$\nu_{\text{calc}}$	$\nu_{\text{obs-calc}}$
3	1	3	2	1	2	6648.9953	6648.9961	-0.0008
3	0	3	2	0	2	7046.7389	7046.7397	-0.0008
3	2	1	2	2	0	7950.6656	7950.6637	0.0020
3	1	2	2	1	1	8190.6968	8190.6976	-0.0008
4	1	4	3	1	3	8758.4613	8758.4615	-0.0002
4	0	4	3	0	3	9041.3421	9041.3419	0.0001
4	2	3	3	2	2	9901.4097	9901.4099	-0.0002
4	3	2	3	3	1	10197.7630	10197.7611	0.0020
4	3	1	3	3	0	10305.8030	10305.8018	0.0012
5	0	5	4	1	4	10688.6395	10688.6396	-0.0001
4	1	3	3	1	2	10731.0110	10731.0117	-0.0008
5	1	5	4	1	4	10815.4033	10815.4034	-0.0001
4	2	2	3	2	1	10855.9752	10855.9742	0.0009
5	0	5	4	0	4	10972.0694	10972.0684	0.0010
5	1	5	4	0	4	11098.8317	11098.8322	-0.0006
5	2	4	4	2	3	12226.2191	12226.2188	0.0003
5	3	3	4	3	2	12761.8734	12761.8740	-0.0006
5	4	2	4	4	1	12769.3923	12769.3928	-0.0006
6	0	6	5	1	5	12782.7884	12782.7886	-0.0003
5	4	1	4	4	0	12787.8043	12787.8046	-0.0003
6	1	6	5	1	5	12835.5010	12835.5005	0.0005

6	0	6	5	0	5	12909.5528	12909.5525	0.0004
6	1	6	5	0	5	12962.2654	12962.2643	0.0011
5	1	4	4	1	3	13070.0370	13070.0366	0.0004
5	3	2	4	3	1	13107.7051	13107.7055	-0.0004
5	2	3	4	2	2	13733.5619	13733.5626	-0.0007
6	2	5	5	2	4	14465.0395	14465.0397	-0.0003
7	1	7	6	1	6	14833.9591	14833.9594	-0.0003
7	0	7	6	0	6	14865.7902	14865.7910	-0.0008
6	1	5	5	1	4	15173.5255	15173.5265	-0.0010
6	3	4	5	3	3	15284.7559	15284.7562	-0.0003
6	4	3	5	4	2	15391.1095	15391.1090	0.0004
6	4	2	5	4	1	15470.1257	15470.1264	-0.0007
6	3	3	5	3	2	16064.9695	16064.9700	-0.0005
6	2	4	5	2	3	16473.8172	16473.8169	0.0003
7	2	6	6	2	5	16621.0906	16621.0910	-0.0004
8	1	8	7	1	7	16821.4131	16821.4130	0.0000
8	0	8	7	0	7	16834.3025	16834.3018	0.0006
7	1	6	6	1	5	17105.1017	17105.1013	0.0004
7	3	5	6	3	4	17737.7479	17737.7481	-0.0002
7	5	3	6	5	2	17939.2584	17939.2581	0.0003
7	5	2	6	5	1	17953.2744	17953.2743	0.0002
7	4	4	6	4	3	18019.9057	18019.9060	-0.0003
7	4	3	6	4	2	18262.0532	18262.0538	-0.0006
8	2	7	7	2	6	18708.3651	18708.3648	0.0003
9	1	9	8	1	8	18803.8709	18803.8708	0.0002
9	0	9	8	0	8	18808.8816	18808.8812	0.0004
8	1	7	7	1	6	18984.7982	18984.7987	-0.0005
7	2	5	6	2	4	19009.7345	19009.7346	-0.0001
7	3	4	6	3	3	19093.5920	19093.5918	0.0002
8	4	5	7	4	4	20629.1659	20629.1653	0.0006
9	2	8	8	2	7	20746.4925	20746.4929	-0.0004
10	1	10	9	1	9	20784.2603	20784.2612	-0.0009
10	0	10	9	0	9	20786.1526	20786.1522	0.0004
9	1	8	8	1	7	20885.2951	20885.2955	-0.0004
8	4	4	7	4	3	21206.5492	21206.5498	-0.0006
8	3	5	7	3	4	22045.4823	22045.4816	0.0008
9	3	7	8	3	6	22367.1521	22367.1520	0.0002
10	2	9	9	2	8	22754.2406	22754.2409	-0.0003
10	1	9	9	1	8	22818.2065	22818.2059	0.0006
9	2	7	8	2	6	23317.5267	23317.5263	0.0003

Table 9: *trans*-2-fluorothiophenol (parent)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	$\nu_{\text{obs}}$	$\nu_{\text{calc}}$	$\nu_{\text{obs-calc}}$
6	3	3	6	2	4	6186.7493	6186.7499	-0.0006
6	2	4	6	1	5	6198.2276	6198.2249	0.0027
5	3	2	5	2	3	6607.0010	6607.0016	-0.0006
3	1	3	2	1	2	6806.4718	6806.4729	-0.0011
3	0	3	2	0	2	7213.9382	7213.9390	-0.0008
4	3	1	4	2	2	7248.0920	7248.0893	0.0027
5	1	4	5	0	5	7631.5280	7631.5266	0.0014
3	1	3	2	0	2	7795.2365	7795.2352	0.0013
4	2	3	4	1	4	7822.1476	7822.1487	-0.0011
7	2	5	7	1	6	8145.8292	8145.8293	-0.0001
3	1	2	2	1	1	8384.1039	8384.1074	-0.0035
4	0	4	3	1	3	8674.8491	8674.8489	0.0002
4	3	2	4	2	3	8682.0670	8682.0688	-0.0018
8	4	4	8	3	5	8683.2005	8683.2000	0.0005
4	1	4	3	1	3	8966.0540	8966.0544	-0.0004
4	0	4	3	0	3	9256.1458	9256.1451	0.0008
4	1	4	3	0	3	9547.3504	9547.3506	-0.0002
4	2	3	3	2	2	10135.5108	10135.5094	0.0014
5	0	5	4	1	4	10941.5266	10941.5268	-0.0002
5	1	5	4	1	4	11071.8951	11071.8949	0.0002
4	2	2	3	2	1	11111.4367	11111.4367	0.0001
5	0	5	4	0	4	11232.7328	11232.7324	0.0004
5	1	5	4	0	4	11363.1007	11363.1005	0.0002
6	4	3	6	3	4	11571.2962	11571.2990	-0.0029
7	4	4	7	3	5	11859.1550	11859.1556	-0.0006
3	2	2	2	1	1	11862.4068	11862.4058	0.0010
5	2	4	4	2	3	12515.5511	12515.5505	0.0006
7	2	6	7	1	7	12762.7072	12762.7087	-0.0016
5	3	3	4	3	2	13063.0756	13063.0756	0.0000
6	0	6	5	1	5	13085.7403	13085.7401	0.0002
6	1	6	5	1	5	13140.0024	13140.0024	0.0000
6	0	6	5	0	5	13216.1083	13216.1082	0.0001
6	1	6	5	0	5	13270.3702	13270.3705	-0.0003
5	1	4	4	1	3	13379.8931	13379.8936	-0.0005
5	3	2	4	3	1	13416.0595	13416.0591	0.0004
4	2	3	3	1	2	13613.8090	13613.8077	0.0013
6	1	5	5	2	4	13769.4405	13769.4409	-0.0004



3	2	1	2	1	2	14046.5868	14046.5869	-0.0001
5	2	3	4	2	2	14057.1461	14057.1468	-0.0008
7	5	2	7	4	3	14203.1702	14203.1700	0.0002
9	3	7	9	2	8	14292.1806	14292.1804	0.0002
8	1	7	8	0	8	14445.3364	14445.3372	-0.0008
8	5	4	8	4	5	14498.2302	14498.2285	0.0018
6	5	1	6	4	2	14518.3737	14518.3724	0.0014
7	5	3	7	4	4	14534.4504	14534.4508	-0.0005
6	5	2	6	4	3	14617.0998	14617.1011	-0.0013
6	2	5	5	2	4	14807.6822	14807.6839	-0.0017
5	2	4	4	1	3	15144.5408	15144.5394	0.0014
7	0	7	6	1	6	15164.4124	15164.4122	0.0003
7	1	7	6	1	6	15185.9262	15185.9268	-0.0006
7	0	7	6	0	6	15218.6758	15218.6745	0.0013
7	1	7	6	0	6	15240.1895	15240.1891	0.0004
6	1	5	5	1	4	15534.0864	15534.0866	-0.0002
6	3	4	5	3	3	15645.7330	15645.7329	0.0001
6	4	3	5	4	2	15754.0689	15754.0690	-0.0001
6	4	2	5	4	1	15834.5862	15834.5851	0.0011
3	3	1	2	2	0	15929.5618	15929.5611	0.0007
3	3	0	2	2	1	16074.1836	16074.1829	0.0007
10	3	8	10	2	9	16121.23809	16121.2385	-0.0004
6	3	3	5	3	2	16442.4701	16442.4701	-0.0001
9	1	8	9	0	9	16571.8413	16571.8408	0.0005
6	2	5	5	1	4	16572.3291	16572.3296	-0.0005
9	2	8	9	1	9	16683.1905	16683.1890	0.0015
6	2	4	5	2	3	16862.7224	16862.7219	0.0006
7	2	6	6	2	5	17015.1502	17015.1498	0.0004
8	0	8	7	1	7	17212.3145	17212.3142	0.0004
8	1	8	7	1	7	17220.5562	17220.5560	0.0002
8	0	8	7	0	7	17233.8287	17233.8288	0.0000
8	1	8	7	0	7	17242.0701	17242.0706	-0.0005
9	6	3	9	5	4	17390.7764	17390.7757	0.0007
7	1	6	6	1	5	17512.0047	17512.0048	-0.0001
9	6	4	9	5	5	17612.7471	17612.7476	-0.0004
8	6	2	8	5	3	17692.1893	17692.1902	-0.0009
8	6	3	8	5	4	17761.0676	17761.0685	-0.0009
7	6	1	7	5	2	17869.4487	17869.4476	0.0011
7	6	2	7	5	3	17886.2849	17886.2847	0.0002
7	3	5	6	3	4	18157.0406	18157.0401	0.0006
8	2	6	7	3	5	18191.1840	18191.1839	0.0001

4	3	2	3	2	1	18230.1581	18230.1579	0.0002
4	2	2	3	1	3	18351.5506	18351.5506	-0.0001
7	5	3	6	5	2	18362.2456	18362.2464	-0.0008
7	5	2	6	5	1	18376.5073	18376.5060	0.0013
7	4	4	6	4	3	18444.8971	18444.8966	0.0004
7	4	3	6	4	2	18691.7075	18691.7083	-0.0008
8	1	7	7	2	6	18894.9436	18894.9426	0.0010
4	3	1	3	2	2	18946.9444	18946.9462	-0.0017
8	2	7	7	2	6	19152.2011	19152.2020	-0.0009
9	0	9	8	1	8	19246.9742	19246.9744	-0.0002
9	1	9	8	1	8	19250.0514	19250.0516	-0.0003
9	0	9	8	0	8	19255.2166	19255.2163	0.0003
9	1	9	8	0	8	19258.2935	19258.2935	-0.0001
8	1	7	7	1	6	19436.3291	19436.3306	-0.0016
7	2	5	6	2	4	19459.6086	19459.6092	-0.0006
7	3	4	6	3	3	19542.4358	19542.4366	-0.0008
8	2	7	7	1	6	19693.5897	19693.5900	-0.0004
5	3	3	4	2	2	20181.7972	20181.7969	0.0004
8	3	6	7	3	5	20576.7211	20576.7219	-0.0008
9	1	8	8	2	7	21124.4594	21124.4606	-0.0011
9	2	8	8	2	7	21238.8861	21238.8859	0.0002
10	0	10	9	1	9	21276.29477	21276.2940	0.0008
10	1	10	9	1	9	21277.42074	21277.4202	0.0005
10	0	10	9	0	9	21279.3712	21279.3712	0.0000
10	1	10	9	0	9	21280.49723	21280.4974	-0.0002
9	1	8	8	1	7	21381.7202	21381.7199	0.0002
9	2	8	8	1	7	21496.1461	21496.1453	0.0007
6	3	4	5	2	3	21770.3832	21770.3829	0.0003
8	2	6	7	2	5	21796.2765	21796.2758	0.0007
4	4	1	3	3	0	21874.7154	21874.7147	0.0006
5	3	2	4	2	3	22227.4962	22227.4960	0.0002
8	3	5	7	3	4	22564.6611	22564.6609	0.0002
9	3	7	8	3	6	22897.0134	22897.0132	0.0001
7	3	5	6	2	4	23064.6993	23064.7011	-0.0018
10	1	9	9	2	8	23245.86526	23245.8650	0.0003
10	2	9	9	2	8	23294.3959	23294.3962	-0.0003
11	0	11	10	1	10	23303.57416	23303.5747	-0.0006
11	0	11	10	0	10	23304.70143	23304.7009	0.0005