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Supplementary tables for the manuscript:

## **Rotational spectra and structures of 2-Fluorophenol and 3-Fluorophenol**

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

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

**Appendix III: Assigned Transitions for 3-Fluorophenol**

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

Table 1. Z-Matrix Structure for *cis*-2FPh

C1						
C2	1	1.39374242				
C3	2	1.38272706	1	122.68632406		
C4	3	1.39667730	2	118.49977736	1	0.00000000
C5	4	1.39579528	3	119.86313589	2	0.00000000
C6	5	1.39523658	4	120.62624794	3	0.00000000
F2	2	1.36130810	1	116.86865137	6	180.00000000
H3	3	1.07970251	2	119.33058765	1	180.00000000
H4	4	1.07955190	3	119.67890615	2	180.00000000
H5	5	1.07999130	4	120.02647178	3	180.00000000
H6	6	1.08029376	5	121.48019015	2	-180.00000000
O1	1	1.36467752	2	121.72263959	5	-180.00000000
H1	12	0.96328683	1	108.06089360	6	180.00000000

Table 2. Z-Matrix Structure for *trans*-2FPh

C1						
C2	1	1.39627902				
C3	2	1.38459746	1	121.79498326		
C4	3	1.39650401	2	119.43579322	1	0.00000000
C5	4	1.39373685	3	119.70959888	2	0.00000000
C6	5	1.39599598	4	120.14176079	3	-0.00000000
F2	2	1.34755758	1	118.54443751	3	-180.00000000
H3	3	1.07981535	2	118.65658297	1	180.00000000
H4	4	1.07956720	3	119.79855834	2	180.00000000
H5	5	1.07989028	4	120.36657494	3	180.00000000
H6	6	1.08279327	5	120.30556501	2	-180.00000000
O1	1	1.36631882	2	117.58066828	5	-180.00000000
H1	12	0.96120966	1	108.37808712	6	0.00000000

Table 3. Z-Matrix Structure for *cis*-3FPh

C1						
C2	1	1.39533198				
C3	2	1.38735013	1	118.34737639		
C4	3	1.38549659	2	122.85194199	1	0.00000000
C5	4	1.39626246	3	117.67898731	2	-0.00000000
C6	5	1.39292803	4	121.18972632	3	0.00000000
H2	2	1.08118792	1	121.89992829	3	-180.00000000
F3	3	1.35383828	2	117.98403328	1	180.00000000
H4	4	1.07864888	3	120.07730358	2	180.00000000
H5	5	1.08016922	4	119.44183124	3	180.00000000
H6	6	1.07943465	5	121.36849415	4	180.00000000
O1	1	1.37043234	2	122.26652817	5	-180.00000000
H1	12	0.96111364	1	109.03546373	6	180.00000000

Table 4. Z-Matrix Structure for *trans*-3FPh

C1						
C2	1	1.39453443				
C3	2	1.38489190	1	118.14348149		
C4	3	1.38792788	2	123.07802263	1	0.00000000
C5	4	1.39419291	3	117.73092764	2	0.00000000
C6	5	1.39499724	4	120.91125123	3	-0.00000000
H2	2	1.07887292	1	120.84842025	3	-180.00000000
F3	3	1.35309512	2	118.13214004	1	180.00000000
H4	4	1.07848637	3	120.08469353	2	180.00000000
H5	5	1.08014948	4	119.62020770	3	180.00000000
H6	6	1.08184369	5	120.29561717	4	180.00000000
O1	1	1.37038087	2	116.66381515	3	180.00000000
H1	12	0.96093437	1	108.67718374	2	180.00000000

## Appendix II: Assigned Transitions for 2-Fluorophenol

Table 1: Cis-2-Fluorophenol (Parent)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	V <sub>obs</sub>	V <sub>obs-calc</sub>
2	1	2	1	1	1	6244.5871	0.0003
6	3	3	6	2	4	6477.6176	0.0003
5	2	3	5	2	4	6610.0988	-0.0015
2	0	2	1	0	1	6774.1239	0.0001
5	2	3	5	1	4	7145.7064	0.0010
2	1	2	1	0	1	7350.5535	0.0006
3	2	2	3	1	3	7538.6076	-0.0004
6	4	2	6	3	3	7752.6488	-0.0003
3	2	2	3	0	3	7759.0422	0.0005
3	3	1	3	2	2	7961.7458	-0.0033
2	1	1	1	1	0	8033.3501	0.0001
4	1	3	4	1	4	8305.4536	0.0010
4	1	3	4	0	4	8374.7420	0.0018
7	3	4	7	2	5	8663.6441	0.0001
4	3	2	4	2	3	8776.8096	-0.0001
5	4	1	5	3	2	8858.2546	-0.0013
3	0	3	2	1	2	8950.4423	0.0006
3	1	3	2	1	2	9170.8752	0.0000
3	0	3	2	0	2	9526.8708	0.0000
4	2	3	4	1	4	9550.9495	0.0000
4	2	3	4	0	4	9620.2369	-0.0002
3	1	3	2	0	2	9747.3048	0.0003
4	4	0	4	3	1	9837.7926	0.0056
6	2	4	6	2	5	9975.1416	0.0005
4	3	2	4	1	3	10022.3063	-0.0004
5	3	3	5	2	4	10125.7121	0.0012
6	2	4	6	1	5	10166.5173	0.0009

4	4	1	4	3	2	10452.4034	-0.0021
5	3	3	5	1	4	10661.3153	-0.0006
5	4	2	5	3	3	10701.0772	0.0029
3	2	2	2	2	1	10708.4474	0.0007
2	2	1	1	1	0	11351.2413	0.0001
6	4	3	6	3	4	11367.6285	0.0007
5	1	4	5	1	5	11370.5070	0.0009
5	1	4	5	0	5	11390.0175	0.0016
3	1	2	2	1	1	11751.2698	0.0002
3	2	1	2	2	0	11890.0233	-0.0003
4	0	4	3	1	3	11900.5514	-0.0003
5	2	4	5	1	5	11906.1116	0.0003
5	2	4	5	0	5	11925.6208	-0.0001
4	1	4	3	1	3	11969.8391	-0.0001
6	3	4	6	2	5	11987.9941	-0.0020
4	0	4	3	0	3	12120.9853	0.0000
6	3	4	6	1	5	12179.3697	-0.0017
4	1	4	3	0	3	12190.2727	-0.0001
6	5	1	6	4	2	12374.0224	0.0011
2	2	0	1	1	1	12610.4687	0.0004
4	1	3	3	2	2	12736.6838	0.0000
5	5	0	5	4	1	13059.0464	-0.0023
2	2	0	1	0	1	13716.4334	-0.0010
4	2	3	3	2	2	13982.1809	0.0001
3	2	2	2	1	1	14026.3414	0.0035
6	1	5	6	1	6	14266.0966	0.0001
6	1	5	6	0	6	14271.2321	-0.0017
6	2	5	6	1	6	14457.4720	0.0001
5	0	5	4	1	4	14673.9251	-0.0001
5	1	5	4	1	4	14693.4348	-0.0002
5	0	5	4	0	4	14743.2128	0.0000
5	1	5	4	0	4	14762.7217	-0.0008
4	3	2	3	3	1	14797.2407	-0.0007
4	1	3	3	1	2	15011.7519	-0.0001
4	3	1	3	3	0	15332.8432	-0.0005
4	2	2	3	2	1	16115.3859	-0.0003
4	2	3	3	1	2	16257.2500	0.0008
5	1	4	4	2	3	16512.9900	-0.0015
5	2	4	4	2	3	17048.5966	0.0000
6	0	6	5	1	5	17378.9809	-0.0001
6	1	6	5	1	5	17384.1187	0.0002
6	0	6	5	0	5	17398.4907	-0.0001
6	1	6	5	0	5	17403.6290	0.0008
5	1	4	4	1	3	17758.4892	0.0006
3	2	1	2	1	2	18255.9045	-0.0006
5	2	4	4	1	3	18294.0938	0.0001

3	3	1	2	2	0	18305.3499	-0.0010
5	3	3	4	3	2	18397.4986	0.0009
5	4	2	4	4	1	18646.1661	-0.0001
3	3	0	2	2	1	18772.9415	-0.0011
5	4	1	4	4	0	18819.8679	0.0004
3	2	1	2	0	2	18832.3336	-0.0007

Table 2: Cis-2-Fluorophenol (13C1)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	V <sub>obs</sub>	V <sub>obs-calc</sub>
2	1	1	1	1	0	8024.6082	-0.0004
3	1	3	2	1	2	9154.9332	-0.0008
3	0	3	2	0	2	9507.5199	0.0009
3	1	3	2	0	2	9723.6338	0.0004
3	1	2	2	1	1	11735.5833	-0.0001
4	0	4	3	1	3	11880.1477	-0.0004
3	2	1	2	2	0	11881.4886	0.0016
4	1	4	3	1	3	11947.6415	-0.0001
4	0	4	3	0	3	12096.2626	0.0000
4	1	4	3	0	3	12163.7564	0.0003
4	2	3	3	2	2	13961.5004	0.0001
5	0	5	4	1	4	14646.4356	0.0000
5	1	5	4	1	4	14665.3195	-0.0003
5	0	5	4	0	4	14713.9293	0.0002
4	1	3	3	1	2	14985.5154	-0.0004
4	2	2	3	2	1	16100.3394	-0.0008

Table 3: Cis-2-Fluorophenol (13C2)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	V <sub>obs</sub>	V <sub>obs-calc</sub>
2	1	1	1	1	0	8025.0245	0.0027
3	1	3	2	1	2	9157.0957	-0.0002
3	0	3	2	0	2	9510.5552	-0.0005
3	1	3	2	0	2	9727.8312	-0.0002
3	1	2	2	1	1	11737.0110	-0.0010
3	2	1	2	2	0	11880.8494	-0.0012
4	0	4	3	1	3	11882.8765	-0.0004
4	1	4	3	1	3	11950.8576	0.0002
4	0	4	3	0	3	12100.1531	0.0003
4	1	4	3	0	3	12168.1329	-0.0002
4	2	3	3	2	2	13963.7703	0.0004
5	0	5	4	1	4	14650.4583	0.0007
5	1	5	4	1	4	14669.5116	-0.0007
5	0	5	4	0	4	14718.4384	0.0005
4	1	3	3	1	2	14989.1005	0.0000
4	2	2	3	2	1	16100.4678	0.0001

Table 4: Cis-2-Fluorophenol (13C3)

$J'$	$K_a'$	$K_c'$	$J''$	$K_a''$	$K_c''$	$V_{obs}$	$V_{obs-calc}$
2	1	1	1	1	0	8010.2878	-0.0005
3	1	3	2	1	2	9119.8964	-0.0014
3	0	3	2	0	2	9462.3696	-0.0008
3	1	3	2	0	2	9665.6763	0.0015
3	1	2	2	1	1	11705.3768	0.0012
4	0	4	3	1	3	11835.3543	0.0004
3	2	1	2	2	0	11874.1291	0.0015
4	1	4	3	1	3	11897.5641	0.0006
4	0	4	3	0	3	12038.6579	-0.0003
4	1	4	3	0	3	12100.8673	-0.0005
4	2	3	3	2	2	13919.3687	0.0009
5	1	5	4	1	4	14601.1739	-0.0009
5	0	5	4	0	4	14646.3262	0.0009
4	1	3	3	1	2	14927.2794	-0.0008
4	2	2	3	2	1	16079.1403	-0.0015

Table 5: Cis-2-Fluorophenol (13C4)

$J'$	$K_a'$	$K_c'$	$J''$	$K_a''$	$K_c''$	$V_{obs}$	$V_{obs-calc}$
2	1	1	1	1	0	7911.0245	0.0010
3	1	3	2	1	2	9060.5126	0.0000
3	0	3	2	0	2	9425.8997	-0.0003
3	1	3	2	0	2	9663.8485	-0.0006
3	1	2	2	1	1	11586.1806	-0.0001
3	2	1	2	2	0	11687.4843	-0.0001
4	0	4	3	1	3	11755.4428	0.0002
4	1	4	3	1	3	11832.6439	-0.0011
4	0	4	3	0	3	11993.3919	0.0001
4	1	4	3	0	3	12070.5941	-0.0001
4	2	3	3	2	2	13795.9491	0.0004
5	0	5	4	1	4	14506.9504	-0.0007
5	1	5	4	1	4	14529.3793	-0.0001
5	0	5	4	0	4	14584.1552	0.0016
4	1	3	3	1	2	14830.7647	0.0003
4	2	2	3	2	1	15857.1757	-0.0005

Table 6: Cis-2-Fluorophenol (13C5)

$J'$	$K_a'$	$K_c'$	$J''$	$K_a''$	$K_c''$	$V_{obs}$	$V_{obs-calc}$
2	1	1	1	1	0	7908.3195	0.0019
3	1	3	2	1	2	9059.6413	0.0004
3	0	3	2	0	2	9426.0274	-0.0005
3	1	3	2	0	2	9665.5423	0.0000
3	1	2	2	1	1	11583.2459	0.0000
3	2	1	2	2	0	11681.8562	-0.0046
4	0	4	3	1	3	11754.1317	0.0002
4	1	4	3	1	3	11832.0280	0.0005
4	0	4	3	0	3	11993.6454	-0.0005
4	1	4	3	0	3	12071.5416	-0.0002
4	2	3	3	2	2	13793.2494	0.0014
5	0	5	4	1	4	14506.2744	-0.0003
5	1	5	4	1	4	14528.9591	0.0013
5	0	5	4	0	4	14584.1695	-0.0011
4	1	3	3	1	2	14829.2424	-0.0012
4	2	2	3	2	1	15850.7404	0.0025

Table 7: Cis-2-Fluorophenol (13C6)

$J'$	$K_a'$	$K_c'$	$J''$	$K_a''$	$K_c''$	$V_{obs}$	$V_{obs-calc}$
2	1	1	1	1	0	8007.2197	0.0019
3	1	3	2	1	2	9117.5717	0.0008
3	0	3	2	0	2	9460.5065	0.0003
3	1	3	2	0	2	9664.4938	-0.0005
3	1	2	2	1	1	11701.4772	0.0009
4	0	4	3	1	3	11832.3021	0.0010
3	2	1	2	2	0	11868.7035	-0.0037
4	1	4	3	1	3	11894.8008	0.0006
4	0	4	3	0	3	12036.2889	-0.0003
4	1	4	3	0	3	12098.7867	-0.0016
4	2	3	3	2	2	13915.1129	0.0008
5	0	5	4	1	4	14580.7896	0.0006
5	0	5	4	0	4	14643.2873	-0.0008
5	1	5	4	1	4	14597.9491	-0.0001
4	1	3	3	1	2	14923.5485	-0.0004
4	2	2	3	2	1	16072.5201	0.0011



### Appendix III: Assigned Transitions for 3-Fluorophenol

Table 1: Trans-3-Fluorophenol (Parent)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	V <sub>obs</sub>	V <sub>obs-calc</sub>
3	1	3	2	1	2	8100.1051	0.0000
7	3	4	7	2	5	8360.4422	0.0002
5	1	4	5	1	5	8378.6420	-0.0013
3	0	3	2	0	2	8614.9223	0.0002
8	3	5	8	2	6	8639.9363	-0.0001
5	1	4	5	0	5	8657.5742	0.0002
6	3	3	6	2	4	8699.7951	0.0000
7	2	5	7	1	6	9032.5156	0.0001
3	2	2	2	2	1	9038.5758	0.0007
5	3	2	5	2	3	9407.1185	0.0006
3	2	1	2	2	0	9462.2282	0.0002
3	1	3	2	0	2	9580.3919	0.0003
9	3	6	9	2	7	9693.3109	0.0002
4	2	3	4	1	4	9805.0715	0.0003
3	1	2	2	1	1	9834.3170	0.0002
4	0	4	3	1	3	10149.5274	0.0004
4	3	1	4	2	2	10175.6749	-0.0003
4	2	3	4	0	4	10352.7213	0.0000
6	2	4	5	3	3	10688.2680	-0.0007
4	1	4	3	1	3	10697.1773	0.0003
3	3	0	3	2	1	10753.0644	0.0002
8	2	6	8	2	7	10872.1859	0.0010
4	0	4	3	0	3	11114.9971	0.0006
6	1	5	6	1	6	11235.2828	0.0003
3	3	1	3	2	2	11275.0804	-0.0001
6	1	5	6	0	6	11367.1988	0.0004
5	2	4	5	1	5	11383.5223	0.0004
8	2	6	8	1	7	11527.4990	-0.0001
4	3	2	4	2	3	11552.0308	-0.0002
5	2	4	5	0	5	11662.4524	0.0000
4	1	4	3	0	3	11662.6464	-0.0001
9	4	5	9	3	6	11704.6882	-0.0004
5	1	4	4	2	3	11810.9487	-0.0001
4	2	3	3	2	2	11963.3869	0.0003
5	3	3	5	2	4	12063.8246	-0.0002
4	3	2	3	3	1	12240.3372	0.0000
4	3	1	3	3	0	12321.0247	0.0005
2	2	1	1	1	0	12460.7695	0.0017
8	3	5	7	4	4	12622.9576	0.0000
8	4	4	8	3	5	12714.8127	-0.0003
6	3	4	6	2	5	12867.5332	0.0000

4	2	2	3	2	1	12898.4134	0.0003
4	1	3	3	1	2	12947.1669	0.0005
5	0	5	4	1	4	12958.4460	0.0000
2	2	0	1	1	1	13155.6036	0.0010
6	2	5	6	1	6	13235.7742	0.0010
5	1	5	4	1	4	13237.3770	0.0003
6	2	5	6	0	6	13367.6891	0.0001
5	0	5	4	0	4	13506.0963	0.0001
7	4	3	7	3	4	13780.1824	0.0004
5	1	5	4	0	4	13785.0264	-0.0003
7	3	5	7	2	6	13995.1229	0.0000
9	2	7	9	2	8	14082.1089	-0.0017
7	1	6	7	1	7	14107.2841	0.0012
7	1	6	7	0	7	14166.6121	-0.0001
9	2	7	9	1	8	14415.9791	0.0003
6	4	2	6	3	3	14630.9171	-0.0009
5	2	4	4	2	3	14815.8275	0.0001
3	2	2	2	1	1	14890.9530	0.0006
5	4	1	5	3	2	15165.7482	-0.0003
7	2	5	6	3	4	15234.4485	-0.0013
7	2	6	7	1	7	15305.9813	-0.0007
5	4	2	4	4	1	15312.7152	0.0000
5	4	1	4	4	0	15323.7588	0.0007
5	3	3	4	3	2	15327.6208	-0.0003
7	2	6	7	0	7	15365.3115	0.0000
4	4	0	4	3	1	15436.3925	0.0001
8	3	6	8	2	7	15448.3718	0.0000
5	4	2	5	3	3	15514.5693	-0.0006
4	4	1	4	3	2	15529.4754	-0.0005
6	4	3	6	3	4	15569.6069	-0.0003
6	1	5	5	2	4	15584.5157	-0.0003
5	3	2	4	3	1	15594.4018	-0.0001
6	0	6	5	1	5	15600.8391	-0.0003
6	1	6	5	1	5	15732.7551	-0.0001
7	4	4	7	3	5	15766.1271	-0.0002
6	0	6	5	0	5	15879.7699	-0.0002
5	1	4	4	1	3	15883.8044	-0.0002
6	1	6	5	0	5	16011.6853	-0.0005
8	3	6	8	1	7	16103.6858	-0.0003
8	4	5	8	3	6	16180.7679	-0.0002
5	2	3	4	2	2	16362.9593	0.0000
8	1	7	8	1	8	16877.3933	-0.0011
9	4	6	9	3	7	16879.2738	-0.0003
8	1	7	8	0	8	16903.1467	-0.0011
4	2	3	3	1	2	17020.0223	0.0001
3	2	1	2	1	2	17174.7821	-0.0004

9	3	7	9	2	8	17199.4539	0.0016
8	2	7	8	1	8	17532.7091	0.0003
9	3	7	9	1	8	17533.3205	0.0001
9	3	6	8	4	5	17557.6172	0.0004
8	2	7	8	0	8	17558.4611	-0.0008
6	2	5	5	2	4	17585.0064	-0.0002
7	0	7	6	1	6	18138.6284	0.0000
7	1	7	6	1	6	18197.9578	0.0000
7	0	7	6	0	6	18270.5441	-0.0001
7	1	7	6	0	6	18329.8736	-0.0001
6	5	2	5	5	1	18361.8593	0.0003
6	5	1	5	5	0	18363.1310	-0.0003
9	5	4	9	4	5	18371.4525	0.0004
6	3	4	5	3	3	18388.7149	0.0000
6	4	3	5	4	2	18443.7521	-0.0001
6	4	2	5	4	1	18491.9659	-0.0002
6	1	5	5	1	4	18589.3944	-0.0001
6	3	3	5	3	2	19026.7966	0.0000
7	1	6	6	2	5	19069.4677	0.0001
8	5	3	8	4	4	19116.8453	0.0004
9	1	8	9	0	9	19537.7316	0.0004
7	5	2	7	4	3	19562.8702	0.0003
9	5	5	9	4	6	19655.8789	-0.0001
8	5	4	8	4	5	19679.8381	0.0002
6	2	4	5	2	3	19734.1192	-0.0001
8	2	6	7	3	5	19749.1491	0.0006
7	5	3	7	4	4	19767.8044	0.0004
6	5	1	6	4	2	19808.1960	0.0002
9	2	8	9	1	9	19860.7115	0.0005
6	5	2	6	4	3	19867.4538	-0.0004
3	3	1	2	2	0	20201.4926	0.0000
7	2	6	6	2	5	20268.1668	0.0000
3	3	0	2	2	1	20327.4550	0.0000
6	2	5	5	1	4	20589.8846	-0.0004
8	0	8	7	1	7	20619.6064	-0.0001
8	1	8	7	1	7	20645.3598	0.0000
8	0	8	7	0	7	20678.9358	-0.0002
8	1	8	7	0	7	20704.6892	-0.0001
7	3	5	6	3	4	21395.7564	-0.0001
7	5	3	6	5	2	21492.6261	-0.0002
7	5	2	6	5	1	21499.4808	-0.0001
7	4	4	6	4	3	21592.2764	-0.0001
7	4	3	6	4	2	21744.8069	0.0001
8	1	7	7	2	6	22216.7725	0.0002
7	2	6	6	1	5	22268.6572	-0.0003
7	3	4	6	3	3	22595.5429	0.0000

8	2	7	7	2	6	22872.0867	0.0002
7	2	5	6	2	4	22934.8962	0.0000
4	3	2	3	2	1	22979.6016	-0.0001
9	0	9	8	1	8	23072.4451	0.0001
9	1	9	8	1	8	23083.3334	0.0001
9	0	9	8	0	8	23098.1982	0.0000
9	1	9	8	0	8	23109.0865	0.0000
8	1	7	7	1	6	23415.4717	0.0001
4	3	1	3	2	2	23609.9038	-0.0004
8	2	7	7	1	6	24070.7854	-0.0003
8	3	6	7	3	5	24325.3356	0.0000
8	5	4	7	5	3	24652.0099	-0.0002
8	5	3	7	5	2	24678.5559	0.0002
8	4	5	7	4	4	24739.9762	0.0000
9	1	8	8	2	7	25077.4675	0.0001
8	4	4	7	4	3	25124.5811	0.0003
5	3	3	4	2	2	25408.8091	-0.0007
9	2	8	8	2	7	25411.3360	0.0004
9	1	8	8	1	7	25732.7819	0.0002
8	2	6	7	2	5	25910.4550	-0.0001

Table 2: Trans-3-Fluorophenol (13C1)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	V <sub>obs</sub>	V <sub>obs-calc</sub>
3	1	3	2	1	2	8066.3245	-0.0002
3	0	3	2	0	2	8580.0618	0.0000
3	1	2	2	1	1	9786.1024	-0.0006
4	0	4	3	1	3	10096.5205	0.0002
4	1	4	3	1	3	10653.8218	-0.0009
4	0	4	3	0	3	11073.2860	0.0000
4	1	4	3	0	3	11630.5883	-0.0001
4	2	3	3	2	2	11908.5712	-0.0006
4	3	1	3	3	0	12258.9664	-0.0013
2	2	1	1	1	0	12449.7165	0.0033
4	2	2	3	2	1	12828.8805	0.0016
4	1	3	3	1	2	12886.3575	0.0001
5	0	5	4	1	4	12899.4806	0.0005
5	1	5	4	1	4	13185.0869	0.0000
5	0	5	4	0	4	13456.7823	-0.0002
5	1	5	4	0	4	13742.3912	0.0017
5	3	2	4	3	1	15512.5115	-0.0003
6	0	6	5	1	5	15535.8899	-0.0005
6	1	6	5	1	5	15671.7967	-0.0011
5	1	4	4	1	3	15814.1628	-0.0007
6	0	6	5	0	5	15821.4978	0.0004
6	1	6	5	0	5	15957.4040	-0.0007

5	2	3	4	2	2	16276.1493	0.0006
6	2	5	5	2	4	17509.2832	-0.0003
7	0	7	6	1	6	18066.8254	-0.0006
7	1	7	6	1	6	18128.3237	0.0007
7	0	7	6	0	6	18202.7331	-0.0003
7	1	7	6	0	6	18264.2298	-0.0004
6	3	4	5	3	3	18300.4898	-0.0009
6	1	5	5	1	4	18514.9592	0.0000
6	2	4	5	2	3	19633.8176	0.0003
7	2	6	6	2	5	20183.8380	0.0003
3	3	1	2	2	0	20184.5969	-0.0006
3	3	0	2	2	1	20308.0438	-0.0011
8	0	8	7	1	7	20540.0624	0.0000
8	1	8	7	1	7	20566.9175	0.0001
8	0	8	7	0	7	20601.5589	-0.0003
8	1	8	7	0	7	20628.4145	0.0002
7	1	6	6	1	5	20992.2214	-0.0008
7	3	5	6	3	4	21295.3989	0.0013
7	3	4	6	3	3	22468.9994	0.0009
8	2	7	7	2	6	22779.8779	0.0011
7	2	5	6	2	4	22825.2911	-0.0016
9	0	9	8	0	8	23011.3786	0.0010

Table 3: Trans-3-Fluorophenol (13C2)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	V <sub>obs</sub>	V <sub>obs-calc</sub>
3	1	3	2	1	2	8086.4330	0.0000
3	0	3	2	0	2	8598.6676	0.0018
3	1	2	2	1	1	9828.7333	0.0010
4	0	4	3	1	3	10148.3623	0.0015
4	1	4	3	1	3	10677.1793	0.0000
4	0	4	3	0	3	11089.0525	0.0007
4	1	4	3	0	3	11617.8738	0.0035
4	2	3	3	2	2	11950.7298	0.0016
2	2	1	1	1	0	12377.6992	0.0048
4	2	2	3	2	1	12900.8429	0.0001
4	1	3	3	1	2	12935.6490	-0.0004
5	0	5	4	1	4	12943.7495	0.0012
5	1	5	4	1	4	13210.5446	0.0021
5	0	5	4	0	4	13472.5666	-0.0002
5	1	5	4	0	4	13739.3590	-0.0019
5	3	3	4	3	2	15318.0232	-0.0001
6	0	6	5	1	5	15574.0603	-0.0001
6	1	6	5	1	5	15699.0484	-0.0017
6	0	6	5	0	5	15840.8536	-0.0010
5	1	4	4	1	3	15861.9398	-0.0009

6	1	6	5	0	5	15965.8447	0.0004
5	2	3	4	2	2	16363.7330	-0.0003
6	2	5	5	2	4	17558.8789	-0.0003
7	0	7	6	1	6	18101.9582	0.0000
7	1	7	6	1	6	18157.6515	0.0001
7	0	7	6	0	6	18226.9466	-0.0012
7	1	7	6	0	6	18282.6409	0.0000
6	3	4	5	3	3	18375.3390	-0.0012
6	1	5	5	1	4	18552.8866	-0.0012
6	2	4	5	2	3	19728.1465	0.0004
3	3	1	2	2	0	20065.2474	-0.0009
3	3	0	2	2	1	20194.0965	-0.0016
7	2	6	6	2	5	20233.5106	0.0016
8	0	8	7	1	7	20574.8466	0.0010
8	1	8	7	1	7	20598.7979	-0.0006
8	0	8	7	0	7	20630.5381	-0.0006
8	1	8	7	0	7	20654.4919	0.0001
7	1	6	6	1	5	21018.5573	-0.0009
7	3	4	6	3	3	22607.0832	0.0009
8	2	7	7	2	6	22828.4539	-0.0004
7	2	5	6	2	4	22917.0678	-0.0011

Table 4: Trans-3-Fluorophenol (13C3)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	V <sub>obs</sub>	V <sub>obs-calc</sub>
3	1	3	2	1	2	8070.9449	-0.0001
3	0	3	2	0	2	8584.8573	0.0007
3	1	2	2	1	1	9792.5319	0.0009
4	0	4	3	1	3	10103.5351	0.0010
4	1	4	3	1	3	10659.7825	0.0004
4	0	4	3	0	3	11079.0999	0.0000
4	1	4	3	0	3	11635.3465	-0.0014
4	2	3	3	2	2	11915.9538	-0.0014
4	3	1	3	3	0	12267.2045	0.0000
4	2	2	3	2	1	12838.0215	-0.0011
4	1	3	3	1	2	12894.5192	0.0001
5	0	5	4	1	4	12907.4413	0.0000
5	1	5	4	1	4	13192.3081	0.0010
5	0	5	4	0	4	13463.6884	-0.0009
5	1	5	4	0	4	13748.5549	-0.0001
6	0	6	5	1	5	15544.7840	0.0000
6	1	6	5	1	5	15680.2444	0.0008
5	1	4	4	1	3	15823.6152	-0.0009
6	1	6	5	0	5	15965.1082	-0.0011
5	2	3	4	2	2	16287.5932	-0.0002
6	2	5	5	2	4	17519.5874	-0.0002

7	0	7	6	1	6	18076.7402	-0.0001
7	1	7	6	1	6	18137.9922	-0.0001
7	0	7	6	0	6	18212.1996	-0.0003
7	1	7	6	0	6	18273.4519	0.0000
6	3	4	5	3	3	18312.2896	-0.0008
6	1	5	5	1	4	18525.2216	0.0004
6	2	4	5	2	3	19647.1246	-0.0005
3	3	1	2	2	0	20188.4323	-0.0014
7	2	6	6	2	5	20195.3797	0.0000
3	3	0	2	2	1	20312.1796	0.0017
8	0	8	7	1	7	20551.0948	0.0013
8	1	8	7	1	7	20577.8237	0.0005
8	0	8	7	0	7	20612.3446	-0.0008
8	1	8	7	0	7	20639.0746	-0.0004
7	1	6	6	1	5	21003.0969	0.0004
7	3	5	6	3	4	21308.8689	0.0002
8	2	7	7	2	6	22792.5670	0.0009
7	2	5	6	2	4	22839.9737	0.0009

Table 5: Trans-3-Fluorophenol (13C4)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	V <sub>obs</sub>	V <sub>obs-calc</sub>
3	1	3	2	1	2	8051.6690	0.0003
3	0	3	2	0	2	8562.3587	-0.0005
3	1	2	2	1	1	9782.3295	0.0011
4	0	4	3	1	3	10098.7621	0.0004
4	1	4	3	1	3	10632.0125	0.0004
4	2	3	3	2	2	11896.5146	0.0026
4	2	2	3	2	1	12836.2434	0.0005
4	1	3	3	1	2	12876.1574	-0.0005
5	0	5	4	1	4	12885.4446	-0.0002
5	0	5	4	0	4	13418.6948	-0.0004
5	1	5	4	0	4	13688.6972	0.0002
6	0	6	5	1	5	15507.3095	-0.0017
6	1	5	5	2	4	15535.2998	0.0003
6	1	6	5	1	5	15634.2581	0.0002
6	0	6	5	0	5	15777.3129	0.0000
5	1	4	4	1	3	15791.9259	0.0000
6	1	6	5	0	5	15904.2595	0.0000
5	2	3	4	2	2	16282.6852	-0.0009
4	2	3	3	1	2	16876.7516	0.0005
6	2	5	5	2	4	17482.0685	-0.0004
7	0	7	6	1	6	18026.4410	-0.0007
7	1	7	6	1	6	18083.2068	-0.0005
7	0	7	6	0	6	18153.3845	-0.0039

7	1	7	6	0	6	18210.1541	0.0000
6	3	4	5	3	3	18289.6859	0.0009
6	1	5	5	1	4	18475.1239	-0.0013
6	2	4	5	2	3	19633.0618	-0.0004
3	3	1	2	2	0	20017.4162	-0.0002
7	2	6	6	2	5	20146.7154	-0.0007
8	0	8	7	1	7	20490.1583	0.0003
8	1	8	7	1	7	20514.6587	0.0009
8	0	8	7	0	7	20546.9244	0.0009
7	1	6	6	1	5	20934.2224	0.0005
7	3	4	6	3	3	22491.1316	-0.0005
8	2	7	7	2	6	22732.2358	0.0005
7	2	5	6	2	4	22810.7470	0.0001
9	0	9	8	1	8	22926.6034	-0.0004
9	1	9	8	1	8	22936.9037	0.0002
9	0	9	8	0	8	22951.1053	0.0016
8	1	7	7	1	6	23261.8254	0.0008

Table 6: Trans-3-Fluorophenol (13C5)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	V <sub>obs</sub>	V <sub>obs-calc</sub>
3	1	3	2	1	2	8053.3818	-0.0006
3	0	3	2	0	2	8559.1972	0.0008
3	1	2	2	1	1	9814.0764	0.0004
4	0	4	3	1	3	10142.0490	0.0006
4	1	4	3	1	3	10628.9592	-0.0007
4	0	4	3	0	3	11026.7839	0.0000
4	1	4	3	0	3	11513.6978	0.0022
4	2	3	3	2	2	11919.3589	0.0015
4	3	1	3	3	0	12305.3898	0.0007
4	2	2	3	2	1	12904.6496	-0.0016
5	0	5	4	1	4	12905.7853	-0.0012
4	1	3	3	1	2	12906.3282	0.0007
5	1	5	4	1	4	13146.0173	0.0000
5	0	5	4	0	4	13392.6975	-0.0006
5	1	5	4	0	4	13632.9276	-0.0013
5	3	3	4	3	2	15293.4112	-0.0001
6	0	6	5	1	5	15508.1338	0.0001
6	1	6	5	1	5	15618.2101	-0.0011
6	0	6	5	0	5	15748.3646	0.0001
5	1	4	4	1	3	15807.4290	-0.0004
6	1	6	5	0	5	15858.4409	-0.0012
6	2	5	5	2	4	17494.9251	-0.0002
7	0	7	6	1	6	18013.1876	0.0008
7	1	7	6	1	6	18061.1731	-0.0018



7	0	7	6	0	6	18123.2648	0.0003
7	1	7	6	0	6	18171.2535	0.0009
6	1	5	5	1	4	18463.4394	-0.0002
6	2	4	5	2	3	19709.8277	0.0004
3	3	0	2	2	1	19887.5177	-0.0001
7	2	6	6	2	5	20149.1550	-0.0001
8	0	8	7	1	7	20467.3069	-0.0001
8	1	8	7	1	7	20487.5042	0.0000
8	0	8	7	0	7	20515.2957	0.0005
7	1	6	6	1	5	20894.6934	-0.0001
8	2	7	7	2	6	22722.8197	0.0000
9	1	9	8	1	8	22905.3488	0.0014

Table 7: Trans-3-Fluorophenol (13C6)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	Vobs	Vobs-calc
3	1	3	2	1	2	8048.7757	0.0010
3	0	3	2	0	2	8559.5681	-0.0001
3	1	2	2	1	1	9776.9722	-0.0006
4	0	4	3	1	3	10092.4712	0.0004
4	1	4	3	1	3	10628.5142	-0.0008
4	0	4	3	0	3	11041.3313	0.0011
4	2	3	3	2	2	11890.9795	0.0017
4	3	1	3	3	0	12250.3749	0.0035
2	2	1	1	1	0	12353.7291	0.0002
4	2	2	3	2	1	12827.5909	0.0029
4	1	3	3	1	2	12869.8039	-0.0001
5	0	5	4	1	4	12879.6182	-0.0011
5	1	5	4	1	4	13151.4697	0.0014
5	0	5	4	0	4	13415.6643	0.0007
5	1	5	4	0	4	13687.5123	-0.0002
6	0	6	5	1	5	15501.8144	-0.0003
6	1	6	5	1	5	15629.8328	0.0002
6	0	6	5	0	5	15773.6621	-0.0014
5	1	4	4	1	3	15785.4246	0.0000
6	1	6	5	0	5	15901.6805	-0.0009
5	2	3	4	2	2	16272.0921	-0.0011
6	2	5	5	2	4	17475.1924	0.0002
7	0	7	6	1	6	18020.9743	-0.0008
7	1	7	6	1	6	18078.3085	-0.0006
7	0	7	6	0	6	18148.9924	-0.0005
7	1	7	6	0	6	18206.3274	0.0003
6	1	5	5	1	4	18469.3423	0.0000
6	2	4	5	2	3	19621.4416	-0.0008
3	3	1	2	2	0	20027.2553	0.0012

7	2	6	6	2	5	20139.5483	-0.0015
3	3	0	2	2	1	20153.8087	-0.0008
8	0	8	7	1	7	20484.4589	0.0022
8	1	8	7	1	7	20509.2407	0.0005
8	0	8	7	0	7	20541.7911	0.0003
7	1	6	6	1	5	20929.3397	-0.0019
8	2	7	7	2	6	22724.9050	0.0008
7	2	5	6	2	4	22799.0613	-0.0019

Table 8: Cis-3-Fluorophenol (Parent)

$J'$	$K_a'$	$K_c'$	$J''$	$K_a''$	$K_c''$	$V_{obs}$	$V_{obs-calc}$
3	1	3	2	1	2	8085.9591	0.0000
3	0	3	2	0	2	8600.8373	0.0002
3	1	2	2	1	1	9810.6286	-0.0001
4	1	4	3	1	3	10679.6308	0.0000
4	0	4	3	0	3	11099.7738	0.0001
4	2	2	3	2	1	12861.6601	0.0000
4	1	3	3	1	2	12918.3886	-0.0002
5	0	5	4	1	4	12931.3847	0.0000
5	1	5	4	1	4	13216.8921	0.0000
5	0	5	4	0	4	13488.8360	0.0000
5	1	5	4	0	4	13774.3438	0.0004
5	2	4	4	2	3	14786.1828	-0.0001
5	3	3	4	3	2	15291.2768	-0.0003
5	3	2	4	3	1	15551.9327	0.0000
6	0	6	5	1	5	15573.7072	0.0002
6	1	6	5	1	5	15709.4840	0.0003
5	1	4	4	1	3	15852.9813	-0.0001
6	0	6	5	0	5	15859.2147	0.0004
6	1	6	5	0	5	15994.9897	-0.0012
5	2	3	4	2	2	16317.6000	0.0002
6	2	5	5	2	4	17552.1319	0.0000
7	1	7	6	1	6	18171.8294	-0.0003
7	0	7	6	0	6	18246.2057	0.0000
6	5	2	5	5	1	18317.5097	0.0009
6	3	4	5	3	3	18346.1713	-0.0001
6	4	3	5	4	2	18398.5112	0.0000
6	4	2	5	4	1	18445.1250	-0.0007
6	1	5	5	1	4	18559.7051	0.0000
6	3	3	5	3	2	18970.9617	0.0000
6	2	4	5	2	3	19683.3824	0.0002
7	2	6	6	2	5	20232.9387	0.0000
8	1	8	7	1	7	20616.2219	0.0000
8	0	8	7	0	7	20650.8256	0.0000

7	1	6	6	1	5	21042.2939	0.0001
7	3	5	6	3	4	21348.3266	0.0000
7	5	2	6	5	1	21446.4207	0.0004
7	4	4	6	4	3	21539.0119	-0.0011
7	4	3	6	4	2	21686.6457	-0.0004
7	3	4	6	3	3	22526.8843	0.0003
8	2	7	7	2	6	22835.0008	0.0006
7	2	5	6	2	4	22882.2222	0.0001
9	1	9	8	1	8	23051.0419	0.0000
9	0	9	8	0	8	23066.4482	0.0000
8	1	7	7	1	6	23387.5320	-0.0002
8	3	6	7	3	5	24274.4923	-0.0001