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Supplementary Information for the Manuscript:

## **Rotational Spectroscopic and *Ab Initio* Investigation of the Rotamer Geometries of 2-Fluoroanisole and 3-Fluoroanisole**

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**Appendix I: Equilibrium Structures From MP2/cc-pVTZ Geometry Optimization Calculations For 2-Fluoroanisole, 3-Fluoroanisole and Anisole**

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**Appendix IV: Ground State Effective Structures ( $r_0$ )**

**Appendix I: Equilibrium Structures From MP2/cc-pVTZ Geometry Optimization Calculations For 2-Fluoroanisole and 3-Fluoroanisole**

Table S1: Z-matrix structure for *anti* 2-fluoroanisole

C1						
C2	1	1.3960526				
C3	2	1.3803630	1	119.4468451		
C4	3	1.4016450	2	121.9670004	1	0.0004664
C5	4	1.3950307	3	118.0477716	2	0.0000000
C6	1	1.3883970	2	119.5851296	3	-0.0004757
H7	1	1.0802054	6	120.5764677	5	179.9996805
H8	2	1.0804857	1	121.9428615	6	-180.0000000
H9	5	1.0789282	4	120.1708388	3	179.9986754
H10	6	1.0807531	1	120.2424707	2	-179.9996431
O11	4	1.3558744	3	116.1243373	2	179.9980177
C12	11	1.4178255	4	115.8656988	3	179.9910559
H13	12	1.0842845	11	105.8297084	4	-179.9866905
H14	12	1.0910067	11	111.2511109	4	-61.1240029
H15	12	1.0910108	11	111.2524973	4	61.1502972
F16	3	1.3402367	2	119.7875899	1	179.9993269

Table S2: Z-matrix structure for nonplanar 2-fluoroanisole

C1						
C2	1	1.3935114				
C3	2	1.3845482	1	119.2613362		
C4	3	1.3976050	2	121.8078190	1	-0.7409953
C5	4	1.3929305	3	118.1631411	2	0.7805768
C6	1	1.3924469	2	119.9554074	3	0.0422383
H7	1	1.0804928	6	120.4390857	5	-179.7562999
H8	2	1.0805155	1	121.9036950	6	179.2114477
H9	5	1.0810828	4	117.7495777	3	179.2730705
H10	6	1.0806111	1	120.2310194	2	-179.7105922

O11	4	1.3666260	3	122.0048374	2	177.9169089
C12	11	1.4294190	4	113.3264048	3	67.7956248
H13	12	1.0851265	11	106.2097864	4	177.8968288
H14	12	1.0879950	11	111.3948290	4	-62.7973005
H15	12	1.0909099	11	110.3028696	4	59.2723168
F16	3	1.3449103	2	119.2334821	1	178.6453178

Table S3: Z-matrix structure for *anti* 3-fluoroanisole

C1						
C2	1	1.3891356				
C3	2	1.3884042	1	117.7177418		
C4	3	1.3806015	2	122.6501315	1	0.0005647
C5	4	1.3977116	3	118.8169454	2	0.0020718
C6	1	1.3957914	2	121.4406906	3	-0.0018475
H7	1	1.0810492	2	119.4566659	3	179.9980390
H8	2	1.0792170	1	122.2094056	6	179.9976671
H9	4	1.0795928	3	120.9488629	2	-179.9944671
H10	6	1.0780239	1	119.4522377	2	179.9904790
F11	3	1.3456702	2	118.8858729	1	-179.9903144
O12	5	1.3600964	4	115.2670238	3	-179.9983725
C13	12	1.4177735	5	116.3031899	4	179.9986512
H14	13	1.0909335	12	111.2597522	5	61.1522422
H15	13	1.0844707	12	105.9109938	5	180.0000000
H16	13	1.0909099	12	111.2625795	5	-61.1434614

Table S4: Z-matrix structure for *syn* 3-fluoroanisole

C1						
C2	1	1.3959547				
C3	2	1.3817574	1	117.6321105		
C4	3	1.3891434	2	123.1030210	1	-0.0013790
C5	4	1.3955901	3	118.2471844	2	0.0000000

C6	1	1.3870089	2	121.0731674	3	0.0019888
H7	1	1.0809107	6	119.4430875	5	179.9996903
H8	2	1.0791478	1	122.2651142	6	-179.9959598
H9	4	1.0778760	3	118.7182620	2	179.9911424
H10	6	1.0801196	1	121.5063041	2	-179.9986874
F11	3	1.3468988	2	119.2080682	1	179.9971741
O12	5	1.3594877	4	123.9554024	3	179.9992549
C13	12	1.4177500	5	116.3663599	4	0.0043780
H14	13	1.0910514	12	111.2475933	5	61.1472094
H15	13	1.0844153	12	105.9588836	5	-179.9948941
H16	13	1.0910193	12	111.2486474	5	-61.1283838

Table S5: Z-matrix structure for anisole

C1						
C2	1	1.3961548				
C3	2	1.3982115	1	119.7972695		
C4	3	1.3876951	2	120.1591616	1	0.0005527
C5	4	1.3960243	3	120.4248867	2	0.0000000
C6	5	1.3895837	4	119.2529818	3	-0.0009162
H7	1	1.0788774	2	121.1616565	3	179.9993373
H8	3	1.0810110	2	118.3922215	1	-179.9994694
H9	4	1.0814423	3	119.3922810	2	179.9995059
H10	5	1.0805809	4	120.4052892	3	179.9996222
H11	6	1.0815877	5	120.0853702	4	-179.9993974
O12	2	1.3627808	1	124.5316734	6	-179.9973750
C13	12	1.4163976	2	116.2956544	1	0.0015310
H14	13	1.0912865	12	111.3402146	2	61.1257160
H15	13	1.0846708	12	105.9869993	2	-179.9973250
H16	13	1.0912848	12	111.3388602	2	-61.1205560

## Appendix II: Assigned Antitiitions for the Isotopologues of 2-Fluoroanisole and 3-Fluoroanisole

Table S6: *anti* 2-fluoroanisole (parent)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
4	4	0	4	3	1	8291.02783	8291.02840	-0.00057
2	2	1	1	1	0	8556.43272	8556.43286	-0.00014
4	0	4	3	1	3	8559.46162	8559.46190	-0.00028
5	2	4	5	1	5	8567.80412	8567.80461	-0.00049
7	3	5	6	4	2	8569.03908	8569.04082	-0.00174
4	4	1	4	3	2	8575.60688	8575.60650	0.00038
4	1	3	3	2	2	8609.81770	8609.81764	0.00006
4	1	4	3	1	3	8658.78646	8658.78703	-0.00057
5	4	2	5	3	3	8666.23954	8666.23962	-0.00008
6	3	4	6	2	5	8795.12628	8795.12609	0.00019
4	0	4	3	0	3	8821.85552	8821.85757	-0.00205
4	1	4	3	0	3	8921.18252	8921.18269	-0.00017
8	5	3	8	4	4	8952.50611	8952.50597	0.00014
6	4	3	6	3	4	8969.64025	8969.63995	0.00030
7	2	5	7	1	6	8993.44961	8993.45039	-0.00078
6	3	3	5	4	2	9219.20182	9219.20126	0.00056
2	2	0	1	1	1	9346.91741	9346.91784	-0.00043
5	2	3	4	3	2	9449.42798	9449.42824	-0.00026
8	3	6	7	4	3	9485.25067	9485.25093	-0.00026
7	4	4	7	3	5	9580.02794	9580.02786	0.00008
9	3	6	9	2	7	9896.97864	9896.97962	-0.00098
7	5	2	7	4	3	9911.81751	9911.81690	0.00061
4	2	3	3	2	2	9979.88978	9979.88957	0.00021
6	1	5	6	0	6	10025.88028	10025.88049	-0.00021
8	4	5	7	5	2	10118.02458	10118.02506	-0.00048
7	3	5	7	2	6	10239.21075	10239.21110	-0.00035
6	2	5	6	1	6	10326.47036	10326.46987	0.00049

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
4	3	2	3	3	1	10439.06846	10439.06760	0.00086
3	2	2	2	1	1	10500.59035	10500.58972	0.00063
8	4	5	8	3	6	10544.59154	10544.59103	0.00051
6	5	1	6	4	2	10548.35470	10548.35601	-0.00131
5	0	5	4	1	4	10618.57047	10618.57034	0.00013
5	1	5	4	1	4	10652.16380	10652.16406	-0.00026
4	3	1	3	3	0	10686.85392	10686.85206	0.00186
5	0	5	4	0	4	10717.89514	10717.89547	-0.00033
5	1	5	4	0	4	10751.48973	10751.48919	0.00054
4	1	3	3	1	2	10774.05022	10774.05013	0.00009
7	5	3	7	4	4	10850.75626	10850.75605	0.00021
6	5	2	6	4	3	10861.33686	10861.33692	-0.00006
5	5	0	5	4	1	10872.94619	10872.94733	-0.00114
5	5	1	5	4	2	10943.49860	10943.49884	-0.00024
8	5	4	8	4	5	11016.67424	11016.67553	-0.00129
10	6	4	10	5	5	11055.29556	11055.29584	-0.00028
4	2	2	3	2	1	11289.32137	11289.32197	-0.00060
8	2	6	8	1	7	11295.30029	11295.30053	-0.00024
9	5	5	9	4	6	11464.45171	11464.45178	-0.00007
5	1	4	4	2	3	11522.05753	11522.05735	0.00018
9	4	6	9	3	7	11850.42262	11850.42201	0.00061
8	3	6	8	2	7	11913.96723	11913.96767	-0.00044
7	1	6	7	0	7	12065.93927	12065.93954	-0.00027
9	6	3	9	5	4	12107.84897	12107.84903	-0.00006
4	2	3	3	1	2	12144.12266	12144.12206	0.00060
9	4	6	8	5	3	12154.41184	12154.41133	0.00051
7	2	6	7	1	7	12182.51170	12182.51239	-0.00069
5	2	4	4	2	3	12235.24984	12235.25026	-0.00042
10	5	6	10	4	7	12263.67511	12263.67536	-0.00025

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
10	3	7	10	2	8	12365.84745	12365.84811	-0.00066
8	4	4	7	5	3	12594.41680	12594.41632	0.00048
6	0	6	5	1	5	12605.10499	12605.10507	-0.00008
6	1	6	5	1	5	12615.71002	12615.71028	-0.00026
6	0	6	5	0	5	12638.69911	12638.69879	0.00032
6	1	6	5	0	5	12649.30387	12649.30400	-0.00013
8	6	2	8	5	3	12790.30485	12790.30508	-0.00023
5	1	4	4	1	3	12892.12942	12892.12928	0.00014
9	6	4	9	5	5	12998.51115	12998.51156	-0.00041
5	3	3	4	3	2	13023.30991	13023.30953	0.00038
10	6	5	10	5	6	13040.71468	13040.71488	-0.00020
8	6	3	8	5	4	13100.06283	13100.06310	-0.00027
6	2	4	5	3	3	13115.16329	13115.16323	0.00006
3	2	1	2	1	2	13156.27733	13156.27697	0.00036
7	6	1	7	5	2	13166.65125	13166.65202	-0.00077
5	4	1	4	4	0	13177.50158	13177.49845	0.00313
7	6	2	7	5	3	13247.79380	13247.79336	0.00044
7	3	4	6	4	3	13291.50700	13291.50722	-0.00022
6	6	0	6	5	1	13365.76214	13365.75973	0.00241
6	6	1	6	5	2	13380.44217	13380.44250	-0.00033
10	4	7	10	3	8	13433.67175	13433.67127	0.00048
9	2	7	9	1	8	13466.01978	13466.01933	0.00045
5	2	4	4	1	3	13605.32224	13605.32219	0.00005
9	3	7	9	2	8	13732.48975	13732.48886	0.00089
5	3	2	4	3	1	13735.73763	13735.73904	-0.00141
3	3	1	2	2	0	13817.67978	13817.67914	0.00064
8	1	7	8	0	8	14041.92960	14041.93149	-0.00189
3	3	0	2	2	1	14062.59802	14062.59709	0.00093
6	1	5	5	2	4	14063.18092	14063.18095	-0.00003



J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
8	2	7	8	1	8	14083.42138	14083.42136	0.00002
5	2	3	4	2	2	14128.40623	14128.40613	0.00010
6	2	5	5	2	4	14374.37524	14374.37554	-0.00030
7	0	7	6	1	6	14563.24061	14563.24073	-0.00012
7	1	7	6	1	6	14566.43738	14566.43802	-0.00064
7	0	7	6	0	6	14573.84571	14573.84594	-0.00023
7	1	7	6	0	6	14577.04327	14577.04322	0.00005
6	2	5	5	1	4	15087.56806	15087.56845	-0.00039
9	7	2	9	6	3	15434.28212	15434.28281	-0.00069
6	3	4	5	3	3	15509.63496	15509.63647	-0.00151
9	7	3	9	6	4	15516.68962	15516.68929	0.00033
10	2	8	10	1	9	15521.30985	15521.30893	0.00092
10	3	8	10	2	9	15625.40620	15625.40548	0.00072
8	7	1	8	6	2	15679.36698	15679.36826	-0.00128
8	7	2	8	6	3	15697.42465	15697.42332	0.00133
6	4	3	5	4	2	15813.03652	15813.03680	-0.00028
7	7	0	7	6	1	15830.75732	15830.75722	0.00010
7	7	1	7	6	2	15833.50635	15833.50689	-0.00054
4	3	2	3	2	1	15968.30036	15968.29985	0.00051
9	1	8	9	0	9	15987.52377	15987.52269	0.00108
9	2	8	9	1	9	16001.44317	16001.44371	-0.00054
7	1	6	6	2	5	16302.71058	16302.71040	0.00018
7	2	6	6	2	5	16422.48047	16422.48054	-0.00007
7	2	5	6	3	4	16501.03523	16501.03470	0.00053
8	0	8	7	1	7	16511.54427	16511.54405	0.00022
8	1	8	7	1	7	16512.47650	16512.47665	-0.00015
8	0	8	7	0	7	16514.74146	16514.74133	0.00013
8	1	8	7	0	7	16515.67412	16515.67393	0.00019
7	1	6	6	1	5	16613.90470	16613.90499	-0.00029

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
6	2	4	5	2	3	16689.04406	16689.04451	-0.00045
7	2	6	6	1	5	16733.67529	16733.67513	0.00016
6	3	3	5	3	2	16880.02942	16880.02975	-0.00033
4	3	1	3	2	2	17144.67708	17144.67707	0.00001
8	3	5	7	4	4	17405.65041	17405.65118	-0.00077
5	3	3	4	2	2	17702.28715	17702.28741	-0.00026
4	2	2	3	1	3	17836.33350	17836.33344	0.00006
9	8	1	9	7	2	18156.53629	18156.53562	0.00067
8	1	7	7	2	6	18370.96332	18370.96316	0.00016
9	0	9	8	1	8	18456.74493	18456.74446	0.00047
9	1	9	8	0	8	18457.94282	18457.94238	0.00044
8	2	7	7	1	6	18533.15576	18533.15575	0.00001
7	2	5	6	2	4	18895.50884	18895.50795	0.00089
4	4	1	3	3	0	18969.47720	18969.47695	0.00025

Table S7: *anti* 2-fluoroanisole (<sup>13</sup>C1)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
3	0	3	2	1	2	6342.64461	6342.64535	-0.00074
3	1	3	2	0	2	7181.27612	7181.27625	-0.00013
4	0	4	3	1	3	8554.82821	8554.82877	-0.00056
4	1	4	3	0	3	8917.88045	8917.88011	0.00034
2	2	0	1	1	1	9344.99296	9344.99349	-0.00053
3	2	2	2	1	1	10498.98170	10498.98197	-0.00027
5	0	5	4	1	4	10613.41676	10613.41670	0.00006
5	1	5	4	1	4	10647.21380	10647.21446	-0.00066
5	0	5	4	0	4	10713.20755	10713.20782	-0.00027
5	1	5	4	0	4	10747.00515	10747.00558	-0.00043
5	1	4	4	2	3	11512.62208	11512.62087	0.00121

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
4	2	3	3	1	2	12141.93170	12141.93297	-0.00127
6	0	6	5	1	5	12599.26385	12599.26434	-0.00049
6	1	6	5	0	5	12643.74545	12643.74622	-0.00077
6	2	4	5	3	3	13098.37179	13098.37174	0.00005
3	2	1	2	1	2	13150.59621	13150.59741	-0.00120
5	2	4	4	1	3	13602.38248	13602.38332	-0.00084
5	2	4	4	1	3	13602.38452	13602.38332	0.00120
3	3	1	2	2	0	13816.68332	13816.68290	0.00042
6	1	5	5	2	4	14054.24581	14054.24562	0.00019
3	3	0	2	2	1	14060.86915	14060.87039	-0.00124
7	0	7	6	1	6	14556.60451	14556.60550	-0.00099
7	1	7	6	0	6	14570.51472	14570.51504	-0.00032
4	3	2	3	2	1	15966.62989	15966.62849	0.00140
7	1	6	6	2	5	16294.04489	16294.04411	0.00078
7	2	5	6	3	4	16484.77835	16484.78081	-0.00246
8	0	8	7	1	7	16504.06265	16504.06238	0.00027
8	1	8	7	0	7	16508.22886	16508.22986	-0.00100
7	2	6	6	1	5	16727.57390	16727.57319	0.00071
4	3	1	3	2	2	17139.71540	17139.71661	-0.00121
5	3	3	4	2	2	17700.43469	17700.43415	0.00054
8	1	7	7	2	6	18362.09711	18362.09713	-0.00002
9	0	9	8	1	8	18448.39320	18448.39504	-0.00184
9	1	9	8	0	8	18449.60425	18449.60548	-0.00123
8	2	7	7	1	6	18525.48835	18525.48782	0.00053
4	4	1	3	3	0	18968.06388	18968.06550	-0.00162
8	2	6	7	3	5	19412.49039	19412.48849	0.00190
5	4	1	4	3	2	21757.45151	21757.45005	0.00146

Table S8: *anti* 2-fluoroanisole (<sup>13</sup>C2)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
3	0	3	2	1	2	6341.59595	6341.59581	0.00014
3	1	3	2	0	2	7164.57891	7164.57941	-0.00050
4	0	4	3	1	3	8546.95058	8546.95226	-0.00168
4	1	4	3	0	3	8900.45469	8900.45508	-0.00039
3	2	2	2	1	1	10464.73018	10464.72569	0.00449
5	0	5	4	1	4	10600.04716	10600.04631	0.00085
5	1	5	4	1	4	10632.47970	10632.47875	0.00095
5	0	5	4	0	4	10696.61400	10696.61457	-0.00057
5	1	5	4	0	4	10729.04722	10729.04701	0.00021
5	1	4	4	2	3	11521.43017	11521.42930	0.00087
4	2	3	3	1	2	12104.28141	12104.28055	0.00086
6	0	6	5	1	5	12581.71610	12581.71681	-0.00071
6	1	6	5	0	5	12624.31680	12624.31699	-0.00019
3	2	1	2	1	2	13130.08523	13130.08321	0.00202
6	2	4	5	3	3	13145.17878	13145.17853	0.00025
5	2	4	4	1	3	13563.14591	13563.14518	0.00073
3	3	1	2	2	0	13764.86688	13764.86718	-0.00030
3	3	0	2	2	1	14012.50476	14012.50422	0.00054
6	1	5	5	2	4	14049.31208	14049.31242	-0.00034
7	0	7	6	1	6	14535.64842	14535.64937	-0.00095
7	1	7	6	0	6	14548.86234	14548.86141	0.00093
4	3	2	3	2	1	15909.85701	15909.85791	-0.00090
7	1	6	6	2	5	16278.08445	16278.08756	-0.00311
8	0	8	7	1	7	16480.05328	16480.05181	0.00147
8	1	8	7	0	7	16483.97783	16483.97800	-0.00017
7	2	5	6	3	4	16513.96042	16513.95970	0.00072
7	2	6	6	1	5	16694.40592	16694.40794	-0.00202
4	3	1	3	2	2	17098.15190	17098.15213	-0.00023
5	3	3	4	2	2	17637.45817	17637.45790	0.00027

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
8	1	7	7	2	6	18338.68959	18338.68920	0.00039
9	0	9	8	1	8	18421.47192	18421.47102	0.00090
9	1	9	8	0	8	18422.60263	18422.60208	0.00055
8	2	7	7	1	6	18494.23184	18494.23148	0.00036
4	4	1	3	3	0	18897.21283	18897.21335	-0.00052
4	4	0	3	3	1	18951.87979	18951.88010	-0.00031
8	2	6	7	3	5	19419.04618	19419.04737	-0.00119
5	4	1	4	3	2	21691.04166	21691.04286	-0.00120

Table S9: *anti* 2-fluoroanisole (<sup>13</sup>C3)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
3	0	3	2	1	2	6285.99879	6285.99837	0.00042
3	1	3	2	0	2	7145.24995	7145.25313	-0.00318
4	1	3	3	2	2	8484.11688	8484.11596	0.00092
4	0	4	3	1	3	8490.03475	8490.03515	-0.00040
2	2	1	1	1	0	8533.83969	8533.84118	-0.00149
4	1	4	3	0	3	8867.19517	8867.19480	0.00037
2	2	0	1	1	1	9308.95018	9308.95140	-0.00122
6	1	5	6	0	6	9932.06482	9932.06575	-0.00093
3	2	2	2	1	1	10464.30394	10464.30075	0.00319
5	0	5	4	1	4	10539.55770	10539.55758	0.00012
5	1	5	4	1	4	10575.58687	10575.58705	-0.00018
5	0	5	4	0	4	10644.36483	10644.36398	0.00085
5	1	5	4	0	4	10680.39290	10680.39344	-0.00054
5	1	4	4	2	3	11390.34745	11390.34716	0.00029
4	2	3	3	1	2	12098.16586	12098.16467	0.00119
6	0	6	5	1	5	12514.64660	12514.64794	-0.00134
6	1	6	5	0	5	12562.23448	12562.23592	-0.00144

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
6	2	4	5	3	3	12893.41089	12893.41211	-0.00122
3	2	1	2	1	2	13067.64412	13067.64578	-0.00166
5	2	4	4	1	3	13548.09199	13548.09155	0.00044
3	3	1	2	2	0	13783.34439	13783.34359	0.00080
6	1	5	5	2	4	13933.14030	13933.13925	0.00105
3	3	0	2	2	1	14019.31469	14019.31689	-0.00220
7	0	7	6	1	6	14460.09568	14460.09571	-0.00003
7	1	7	6	0	6	14475.19541	14475.19503	0.00038
4	3	2	3	2	1	15922.31520	15922.31546	-0.00026
7	1	6	6	2	5	16172.26974	16172.26892	0.00082
7	2	5	6	3	4	16279.45360	16279.45302	0.00058
8	0	8	7	1	7	16395.09793	16395.09729	0.00064
8	1	8	7	0	7	16399.68660	16399.68746	-0.00086
7	2	6	6	1	5	16633.77292	16633.77372	-0.00080
4	3	1	3	2	2	17058.22221	17058.22142	0.00079
5	3	3	4	2	2	17651.21907	17651.21930	-0.00023
8	1	7	7	2	6	18234.86106	18234.86047	0.00059
9	0	9	8	1	8	18326.74047	18326.74023	0.00024
9	1	9	8	0	8	18328.09136	18328.09293	-0.00157
8	2	7	7	1	6	18411.51019	18411.50974	0.00045
4	4	1	3	3	0	18921.86705	18921.86616	0.00089
4	4	0	3	3	1	18972.47627	18972.47614	0.00013
8	2	6	7	3	5	19220.44035	19220.43925	0.00110
5	4	1	4	3	2	21678.15632	21678.15573	0.00059

Table S10: *anti* 2-fluoroanisole ( $^{13}\text{C4}$ )

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	$\nu_{\text{obs}}/\text{MHz}$	$\nu_{\text{calc}}/\text{MHz}$	$\nu_{\text{obs-calc}}/\text{MHz}$
6	1	6	5	0	5	12519.37022	12519.37023	-0.00001
6	0	6	5	1	5	12469.21588	12469.21644	-0.00056
5	1	4	4	2	3	11313.96692	11313.96702	-0.00010
5	0	5	4	1	4	10499.25593	10499.25649	-0.00056
3	3	1	2	2	0	13778.98470	13778.98509	-0.00039
3	3	0	2	2	1	14009.20419	14009.20495	-0.00076
5	2	4	4	1	3	13527.59413	13527.59281	0.00132
4	2	3	3	1	2	12083.32926	12083.32723	0.00203
5	1	5	4	0	4	10646.04233	10646.04615	-0.00382
7	0	7	6	1	6	14408.60769	14408.60661	0.00108
7	1	7	6	0	6	14424.69655	14424.69662	-0.00007
4	0	4	3	1	3	8453.46807	8453.46787	0.00020
2	2	1	1	1	0	8530.23265	8530.23362	-0.00097
4	1	4	3	0	3	8842.22012	8842.22147	-0.00135
3	2	2	2	1	1	10453.87669	10453.87629	0.00040
3	2	1	2	1	2	13024.71578	13024.71389	0.00189
6	1	5	5	2	4	13861.43207	13861.43117	0.00090
7	1	6	6	2	5	16103.63302	16103.63120	0.00182
8	0	8	7	1	7	16337.08954	16337.09076	-0.00122
8	1	8	7	0	7	16342.03572	16342.03620	-0.00048
7	2	6	6	1	5	16588.13503	16588.13339	0.00164
4	3	1	3	2	2	17022.67397	17022.67647	-0.00250
5	3	3	4	2	2	17640.61684	17640.61254	0.00430
8	1	7	7	2	6	18165.41880	18165.41761	0.00119
9	0	9	8	1	8	18262.02168	18262.02287	-0.00119
9	1	9	8	0	8	18263.49582	18263.49635	-0.00053
4	4	1	3	3	0	18915.58820	18915.58900	-0.00080
4	4	0	3	3	1	18964.26958	18964.27106	-0.00148
5	0	5	4	0	4	10608.17874	10608.17718	0.00156

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
5	1	5	4	1	4	10537.12434	10537.12545	-0.00111
3	0	3	2	1	2	6252.29370	6252.29542	-0.00172
3	1	3	2	0	2	7128.76265	7128.76271	-0.00006
8	2	6	7	3	5	19101.67824	19101.67809	0.00015
5	4	1	4	3	2	21651.23016	21651.23081	-0.00065

Table S11: *anti* 2-fluoroanisole (<sup>13</sup>C5)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
6	1	6	5	0	5	12534.32705	12534.32683	0.00022
6	0	6	5	1	5	12494.22648	12494.23004	-0.00356
5	0	5	4	1	4	10528.08273	10528.08356	-0.00083
3	3	1	2	2	0	13628.79298	13628.79257	0.00041
3	3	0	2	2	1	13879.59631	13879.59507	0.00124
3	2	2	2	1	1	10367.62992	10367.62916	0.00076
5	1	5	4	0	4	10650.79748	10650.79830	-0.00082
4	2	3	3	1	2	11994.37560	11994.37253	0.00307
5	2	4	4	1	3	13443.71669	13443.71353	0.00316
7	0	7	6	1	6	14433.73618	14433.73488	0.00130
7	1	7	6	0	6	14446.03938	14446.04011	-0.00073
4	0	4	3	1	3	8492.53564	8492.53583	-0.00019
4	1	4	3	0	3	8832.40720	8832.40941	-0.00221
5	1	4	4	2	3	11472.27030	11472.27131	-0.00101
6	1	5	5	2	4	13969.73623	13969.73631	-0.00008
7	1	6	6	2	5	16173.20464	16173.20435	0.00029
8	0	8	7	1	7	16364.19297	16364.19317	-0.00020
8	1	8	7	0	7	16367.81161	16367.81165	-0.00004
7	2	5	6	3	4	16463.94031	16463.93956	0.00075
7	2	6	6	1	5	16566.39464	16566.39579	-0.00115



J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
4	3	1	3	2	2	16958.06930	16958.06996	-0.00066
5	3	3	4	2	2	17467.17760	17467.17430	0.00330
8	1	7	7	2	6	18213.86767	18213.86747	0.00020
9	0	9	8	1	8	18291.85452	18291.85471	-0.00019
9	1	9	8	0	8	18292.88566	18292.88625	-0.00059
8	2	7	7	1	6	18359.13838	18359.13701	0.00137
4	4	1	3	3	0	18710.79758	18710.79992	-0.00234
4	4	0	3	3	1	18766.89685	18766.89961	-0.00276
5	0	5	4	0	4	10620.19188	10620.19439	-0.00251
5	1	5	4	1	4	10558.68824	10558.68747	0.00077
3	0	3	2	1	2	6307.22503	6307.22252	0.00251
3	1	3	2	0	2	7106.46245	7106.46097	0.00148
8	2	6	7	3	5	19325.38036	19325.37956	0.00080
5	4	1	4	3	2	21495.99812	21495.99848	-0.00036

Table S12: *anti* 2-fluoroanisole (<sup>13</sup>C6)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
3	0	3	2	1	2	6342.42530	6342.42575	-0.00045
3	1	3	2	0	2	7139.32589	7139.32610	-0.00021
4	0	4	3	1	3	8537.09907	8537.09954	-0.00047
4	1	4	3	0	3	8874.77764	8874.78044	-0.00280
3	2	2	2	1	1	10410.99145	10410.99270	-0.00125
5	0	5	4	1	4	10581.78348	10581.78289	0.00059
5	1	5	4	1	4	10611.98844	10611.98936	-0.00092
5	0	5	4	0	4	10673.04340	10673.04326	0.00014
5	1	5	4	0	4	10703.24999	10703.24972	0.00027
5	1	4	4	2	3	11540.80032	11540.80084	-0.00052
4	2	3	3	1	2	12045.49924	12045.49747	0.00177

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
6	0	6	5	1	5	12557.25871	12557.25769	0.00102
6	1	6	5	0	5	12596.79994	12596.79869	0.00125
6	2	4	5	3	3	13229.93718	13229.93413	0.00305
5	2	4	4	1	3	13502.46009	13502.45921	0.00088
3	3	1	2	2	0	13682.65421	13682.65452	-0.00031
3	3	0	2	2	1	13936.43911	13936.43966	-0.00055
6	1	5	5	2	4	14046.30868	14046.30789	0.00079
7	0	7	6	1	6	14506.27346	14506.27321	0.00025
7	1	7	6	0	6	14518.36218	14518.36287	-0.00069
4	3	2	3	2	1	15820.08503	15820.08524	-0.00021
7	1	6	6	2	5	16257.46687	16257.47068	-0.00381
8	0	8	7	1	7	16446.34074	16446.34131	-0.00057
8	1	8	7	0	7	16449.88323	16449.88326	-0.00003
7	2	5	6	3	4	16569.29882	16569.30098	-0.00216
7	2	6	6	1	5	16645.66760	16645.66875	-0.00115
4	3	1	3	2	2	17035.42327	17035.42621	-0.00294
5	3	3	4	2	2	17537.87730	17537.87144	0.00586
8	1	7	7	2	6	18306.50296	18306.50154	0.00142
9	0	9	8	1	8	18383.65491	18383.65556	-0.00065
9	1	9	8	0	8	18384.66215	18384.66155	0.00060
8	2	7	7	1	6	18449.36275	18449.36347	-0.00072
4	4	1	3	3	0	18784.86770	18784.86798	-0.00028
4	4	0	3	3	1	18841.89660	18841.89749	-0.00089
8	2	6	7	3	5	19436.82746	19436.82580	0.00166
5	4	1	4	3	2	21587.90760	21587.90705	0.00055

Table S13: *anti* 2-fluoroanisole (<sup>13</sup>C7)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
3	0	3	2	1	2	6205.71871	6205.71765	0.00106
3	1	3	2	0	2	7103.45598	7103.45330	0.00268
4	0	4	3	1	3	8401.81662	8401.81786	-0.00124
4	1	4	3	0	3	8805.20293	8805.20419	-0.00126
3	2	2	2	1	1	10434.04310	10434.04400	-0.00090
5	0	5	4	1	4	10441.62519	10441.62559	-0.00040
5	1	5	4	1	4	10481.88506	10481.88538	-0.00032
5	0	5	4	0	4	10555.80566	10555.80560	0.00006
5	1	5	4	0	4	10596.06422	10596.06540	-0.00118
5	1	4	4	2	3	11209.96377	11209.96455	-0.00078
4	2	3	3	1	2	12056.89233	12056.89070	0.00163
6	0	6	5	1	5	12403.91037	12403.91010	0.00027
6	1	6	5	0	5	12457.41370	12457.41289	0.00081
5	2	4	4	1	3	13493.25361	13493.25493	-0.00132
6	1	5	5	2	4	13761.48321	13761.48289	0.00032
3	3	1	2	2	0	13764.63104	13764.62992	0.00112
3	3	0	2	2	1	13987.65873	13987.65850	0.00023
7	0	7	6	1	6	14334.46100	14334.46176	-0.00076
7	1	7	6	0	6	14351.86203	14351.86370	-0.00167
7	2	5	6	3	4	15967.28438	15967.28412	0.00026
7	1	6	6	2	5	16006.24942	16006.25032	-0.00090
8	0	8	7	1	7	16253.51980	16253.51827	0.00153
8	1	8	7	0	7	16258.94201	16258.94069	0.00132
7	2	6	6	1	5	16520.53148	16520.53063	0.00085
4	3	1	3	2	2	16967.68999	16967.69038	-0.00039
5	3	3	4	2	2	17615.79199	17615.79010	0.00189
8	1	7	7	2	6	18065.92550	18065.92412	0.00138
9	0	9	8	1	8	18168.76789	18168.77053	-0.00264
9	1	9	8	0	8	18170.40831	18170.40836	-0.00005

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
8	2	7	7	1	6	18268.04170	18268.04091	0.00079
4	4	1	3	3	0	18895.56140	18895.56287	-0.00147
8	2	6	7	3	5	18937.94938	18937.94876	0.00062
4	4	0	3	3	1	18941.89286	18941.89224	0.00062
5	4	1	4	3	2	21603.93601	21603.93753	-0.00152

Table S14: *anti* 2-fluoroanisole (<sup>18</sup>O)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
3	0	3	2	1	2	6230.42558	6230.42691	-0.00133
3	1	3	2	0	2	7124.30394	7124.30482	-0.00088
3	2	2	2	1	1	10459.99395	10459.99031	0.00364
5	0	5	4	1	4	10477.72494	10477.72671	-0.00177
5	1	5	4	0	4	10630.42795	10630.42737	0.00058
6	0	6	5	1	5	12445.95985	12445.96119	-0.00134
6	1	6	5	0	5	12498.67176	12498.67022	0.00154
5	2	4	4	1	3	13529.17200	13529.17547	-0.00347
3	3	1	2	2	0	13795.67114	13795.67101	0.00013
6	1	5	5	2	4	13815.39521	13815.39422	0.00099
3	3	0	2	2	1	14021.00940	14021.01003	-0.00063
7	0	7	6	1	6	14382.71260	14382.70843	0.00417
7	1	7	6	0	6	14399.78896	14399.79063	-0.00167
8	0	8	7	1	7	16308.09517	16308.09492	0.00025
8	1	8	7	0	7	16313.40047	16313.39866	0.00181
9	0	9	8	1	8	18229.73681	18229.73721	-0.00040
9	1	9	8	0	8	18231.33197	18231.33348	-0.00151
8	2	6	7	3	5	19019.10936	19019.10981	-0.00045

Table S15: *anti* 3-fluoroanisole (parent)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
4	2	2	3	2	1	8021.76202	8021.76148	0.00054
2	2	1	2	1	2	8284.61204	8284.61137	0.00067
4	1	3	3	1	2	8327.64847	8327.64848	-0.00001
10	2	8	10	1	9	8465.80519	8465.80534	-0.00015
3	2	2	3	1	3	8679.52197	8679.52393	-0.00196
7	1	6	6	2	5	8953.56817	8953.56776	0.00041
5	1	5	4	1	4	9107.46658	9107.46663	-0.00005
4	2	3	4	1	4	9211.39851	9211.40055	-0.00204
8	1	7	8	0	8	9252.24356	9252.24457	-0.00101
4	1	4	3	0	3	9256.96276	9256.96305	-0.00029
5	0	5	4	0	4	9474.34241	9474.34113	0.00128
11	2	9	11	1	10	9681.07510	9681.07433	0.00077
5	2	4	4	2	3	9778.59092	9778.59037	0.00055
5	4	2	4	4	1	9861.21097	9861.20823	0.00274
5	4	1	4	4	0	9861.46144	9861.46410	-0.00266
5	3	3	4	3	2	9875.38909	9875.38981	-0.00072
5	2	4	5	1	5	9882.52442	9882.52429	0.00013
5	3	2	4	3	1	9893.00596	9893.00635	-0.00039
12	3	9	12	2	10	9987.41968	9987.42018	-0.00050
6	0	6	5	1	5	10004.74900	10004.74948	-0.00048
11	3	8	1	2	9	10058.50724	10058.50689	0.00035
5	2	3	4	2	2	10123.89880	10123.89859	0.00021
13	3	10	13	2	11	10207.24379	10207.24330	0.00049
10	3	7	10	2	8	10363.31007	10363.30969	0.00038
5	1	4	4	1	3	10368.78985	10368.79023	-0.00038
10	2	8	9	3	7	10678.80922	10678.80944	-0.00022
5	1	5	4	0	4	10688.85427	10688.85495	-0.00068
5	1	5	4	0	4	10688.85437	10688.85495	-0.00058
6	2	5	6	1	6	10693.28012	10693.27948	0.00064

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
9	1	8	9	1	9	10800.13065	10800.13016	0.00049
9	3	6	9	2	7	10828.86401	10828.86366	0.00035
6	1	6	5	1	5	10889.73606	10889.73661	-0.00055
9	1	8	9	0	9	11068.22519	11068.22505	0.00014
12	2	10	12	1	11	11195.25674	11195.25631	0.00043
6	0	6	5	0	5	11219.26317	11219.26331	-0.00014
8	3	5	8	2	6	11372.03461	11372.03475	-0.00014
8	1	7	7	2	6	11608.14172	11608.14150	0.00022
7	2	6	7	1	7	11641.13066	11641.13067	-0.00001
6	2	5	5	2	4	11700.49131	11700.49180	-0.00049
2	2	1	1	1	0	11700.99942	11700.99856	0.00086
6	5	2	5	5	1	11830.47044	11830.46952	0.00092
6	5	1	5	5	0	11830.47669	11830.48045	-0.00376
6	4	3	5	4	2	11846.74903	11846.74736	0.00167
6	4	2	5	4	1	11847.89378	11847.89414	-0.00036
6	3	4	5	3	3	11864.04622	11864.04612	0.00010
6	3	3	5	3	2	11910.39161	11910.39218	-0.00057
7	3	4	7	2	5	11910.73414	11910.73371	0.00043
2	2	0	1	1	1	11975.38793	11975.38744	0.00049
7	0	7	6	1	6	12040.84006	12040.84046	-0.00040
6	1	6	5	0	5	12104.25027	12104.25043	-0.00016
7	2	6	7	0	7	12256.93706	12256.93745	-0.00039
6	2	4	5	2	3	12263.96178	12263.96178	0.00000
6	3	3	6	2	4	12377.47039	12377.47024	0.00015
6	1	5	5	1	4	12378.10558	12378.10601	-0.00043
7	1	7	6	1	6	12656.64682	12656.64723	-0.00041
8	2	7	8	1	8	12719.98516	12719.98398	0.00118
5	3	2	5	2	3	12731.04001	12731.03983	0.00018
10	1	9	10	1	10	12815.90355	12815.90354	0.00001

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
7	0	7	6	0	6	12925.82737	12925.82758	-0.00021
4	3	1	4	2	2	12961.93172	12961.93207	-0.00035
13	2	11	13	1	12	12964.98122	12964.98127	-0.00005
10	1	9	10	0	10	12986.05974	12986.05941	0.00033
3	3	0	3	2	1	13087.91461	13087.91436	0.00025
8	2	7	8	0	8	13132.48847	13132.48919	-0.00072
4	3	2	4	2	3	13228.68534	13228.68665	-0.00131
5	3	3	5	2	4	13325.48641	13325.48610	0.00031
3	2	2	2	1	1	13409.19150	13409.18975	0.00175
6	3	4	6	2	5	13489.04058	13489.04042	0.00016
7	1	7	6	0	6	13541.63421	13541.63436	-0.00015
7	2	6	6	2	5	13604.49850	13604.49843	0.00007
11	2	9	10	3	8	13726.56058	13726.56068	-0.00010
7	3	5	7	2	6	13738.61519	13738.61619	-0.00100
7	6	2	6	6	1	13800.02445	13800.02371	0.00074
7	6	1	6	6	0	13800.02445	13800.02413	0.00032
7	5	3	6	5	2	13813.99187	13813.98805	0.00382
7	5	2	6	5	1	13814.04545	13814.04801	-0.00256
7	4	4	6	4	3	13838.98649	13838.98633	0.00016
7	4	3	6	4	2	13842.78285	13842.78353	-0.00068
7	3	5	6	3	4	13854.07446	13854.07420	0.00026
9	2	8	9	1	9	13920.09939	13920.09938	0.00001
7	3	4	6	3	3	13955.98867	13955.98831	0.00036
8	0	8	7	1	7	13997.02744	13997.02761	-0.00017
8	3	6	8	2	7	14092.05044	14092.05091	-0.00047
9	1	8	8	2	7	14230.57577	14230.57563	0.00014
3	2	1	2	1	2	14268.91129	14268.90967	0.00162
7	1	6	6	1	5	14345.18305	14345.18305	0.00000
8	1	8	7	1	7	14409.53314	14409.53283	0.00031

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
7	2	5	6	2	4	14422.72483	14422.72484	-0.00001
9	3	7	9	2	8	14564.47085	14564.47198	-0.00113
8	0	8	7	0	7	14612.83441	14612.83439	0.00002
4	2	3	3	1	2	14987.07860	14987.07785	0.00075
8	1	8	7	0	7	15025.33953	15025.33961	-0.00008
10	3	8	10	2	9	15167.27939	15167.27926	0.00013
10	2	9	10	1	10	15228.58901	15228.58990	-0.00089
13	4	9	13	3	10	15273.80176	15273.80077	0.00099
8	2	7	7	2	6	15488.38686	15488.38613	0.00073
8	7	1	7	7	0	15769.77154	15769.77214	-0.00060
8	7	2	7	7	1	15769.77154	15769.77213	-0.00059
8	6	3	7	6	2	15782.11262	15782.11117	0.00145
8	6	2	7	6	1	15782.11262	15782.11390	-0.00128
8	5	4	7	5	3	15802.92661	15802.92583	0.00078
8	5	3	7	5	2	15803.16436	15803.16466	-0.00030
8	4	5	7	4	4	15838.27643	15838.27680	-0.00037
8	3	6	7	3	5	15841.82090	15841.82085	0.00005
8	4	4	7	4	3	15848.61196	15848.61197	-0.00001
9	0	9	8	1	8	15882.33501	15882.33456	0.00045
11	3	9	11	2	10	15907.41967	15907.41893	0.00074
12	4	8	12	3	9	16031.83003	16031.83008	-0.00005
8	3	5	7	3	4	16038.33392	16038.33408	-0.00016
9	1	9	8	1	8	16150.42890	16150.42945	-0.00055
8	1	7	7	1	6	16259.07232	16259.07217	0.00015
9	0	9	8	0	8	16294.84030	16294.83978	0.00052
5	2	4	4	1	3	16438.02030	16438.01974	0.00056
9	1	9	8	0	8	16562.93388	16562.93467	-0.00079
9	1	9	8	0	8	16562.93490	16562.93467	0.00023
8	2	6	7	2	5	16577.03262	16577.03304	-0.00042



J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
11	2	10	11	1	11	16630.39740	16630.39660	0.00080
11	4	7	11	3	8	16717.09544	16717.09626	-0.00082
11	2	10	11	0	11	16736.38783	16736.38735	0.00048
10	1	9	9	2	8	16777.47670	16777.47607	0.00063
12	3	10	12	2	11	16786.96712	16786.96786	-0.00074
4	2	2	3	1	3	16793.63695	16793.63751	-0.00056
12	2	10	11	3	9	16803.84191	16803.84212	-0.00021
12	1	11	12	0	12	16887.37795	16887.37850	-0.00055
10	4	6	10	3	7	17280.94794	17280.94776	0.00018
9	2	8	8	2	7	17350.54489	17350.54485	0.00004
9	4	5	9	3	6	17705.93359	17705.93356	0.00003
10	0	10	9	1	9	17711.51596	17711.51604	-0.00008
9	7	3	8	7	2	17750.89266	17750.89363	-0.00097
9	7	2	8	7	1	17750.89266	17750.89374	-0.00108
9	6	4	8	6	3	17768.47901	17768.47835	0.00066
9	6	3	8	6	2	17768.49187	17768.49104	0.00083
6	2	5	5	1	4	17769.72070	17769.72130	-0.00060
9	5	5	8	5	4	17798.00648	17798.00691	-0.00043
9	5	4	8	5	3	17798.77787	17798.77825	-0.00038
13	3	11	13	2	12	17803.06393	17803.06395	-0.00002
9	3	7	8	3	6	17822.96600	17822.96592	0.00008
9	4	6	8	4	5	17844.34938	17844.34947	-0.00009
9	4	5	8	4	4	17868.77871	17868.77869	0.00002
10	1	10	9	1	9	17881.67229	17881.67191	0.00038
10	0	10	9	0	9	17979.61134	17979.61093	0.00041

Table S16: *anti* 3-fluoroanisole (<sup>13</sup>C1)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
4	1	3	3	1	2	8315.77786	8315.77664	0.00122
5	1	5	4	1	4	9095.90716	9095.90818	-0.00102
4	1	4	3	0	3	9249.66572	9249.66602	-0.00030
5	0	5	4	0	4	9462.49567	9462.49655	-0.00088
5	2	4	4	2	3	9765.29269	9765.29290	-0.00021
5	2	3	4	2	2	10108.93605	10108.93667	-0.00062
5	1	4	4	1	3	10354.17876	10354.17803	0.00073
5	1	5	4	0	4	10679.90187	10679.90181	0.00006
6	1	6	5	1	5	10876.04255	10876.04137	0.00118
6	0	6	5	0	5	11205.60895	11205.60875	0.00020
6	2	5	5	2	4	11684.70883	11684.70879	0.00004
6	3	3	5	3	2	11893.45629	11893.45727	-0.00098
7	0	7	6	1	6	12022.52240	12022.52288	-0.00048
6	1	6	5	0	5	12093.44735	12093.44664	0.00071
6	2	4	5	2	3	12245.63289	12245.63140	0.00149
6	1	5	5	1	4	12360.94045	12360.94037	0.00008
7	1	7	6	1	6	12640.86775	12640.86827	-0.00052
7	0	7	6	0	6	12910.36119	12910.36077	0.00042
7	1	7	6	0	6	13528.70516	13528.70616	-0.00100
7	2	6	6	2	5	13586.31919	13586.31905	0.00014
7	4	4	6	4	3	13819.60328	13819.60466	-0.00138
7	4	3	6	4	2	13823.36341	13823.36193	0.00148
7	3	5	6	3	4	13834.72179	13834.72140	0.00039
7	3	4	6	3	3	13935.85797	13935.85812	-0.00015
8	0	8	7	1	7	13977.12194	13977.12166	0.00028
7	1	6	6	1	5	14325.71338	14325.71381	-0.00043
8	1	8	7	1	7	14391.70791	14391.70838	-0.00047
7	2	5	6	2	4	14401.13586	14401.13589	-0.00003
8	0	8	7	0	7	14595.46789	14595.46705	0.00084

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
8	1	8	7	0	7	15010.05441	15010.05377	0.00064
8	2	7	7	2	6	15467.90702	15467.90668	0.00034
8	4	5	7	4	4	15816.02412	15816.02356	0.00056
8	3	6	7	3	5	15819.73659	15819.73694	-0.00035
8	4	4	7	4	3	15826.25009	15826.25065	-0.00056
9	0	9	8	1	8	15860.88672	15860.88660	0.00012
8	3	5	7	3	4	16014.78940	16014.79267	-0.00327
9	1	9	8	1	8	16130.58253	16130.58213	0.00040
8	1	7	7	1	6	16237.60164	16237.60158	0.00006
9	0	9	8	0	8	16275.47309	16275.47332	-0.00023
5	2	4	4	1	3	16429.40540	16429.40544	-0.00004
9	1	9	8	0	8	16545.16874	16545.16885	-0.00011
8	2	6	7	2	5	16552.41159	16552.41051	0.00108
9	2	8	8	2	7	17327.86342	17327.86297	0.00045
10	0	10	9	1	9	17688.48385	17688.48301	0.00084
6	2	5	5	1	4	17759.93612	17759.93620	-0.00008
9	4	6	8	4	5	17819.20522	17819.20492	0.00030
9	4	5	8	4	4	17843.38111	17843.38074	0.00037
10	1	10	9	1	9	17859.80986	17859.81083	-0.00097
10	0	10	9	0	9	17958.17831	17958.17854	-0.00023

Table S17: *anti* 3-fluoroanisole (<sup>13</sup>C2)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
4	2	2	3	2	1	8018.00635	8018.00390	0.00245
4	1	3	3	1	2	8322.68963	8322.68948	0.00015
5	1	5	4	1	4	9094.88861	9094.88845	0.00016
5	0	5	4	0	4	9460.37507	9460.37579	-0.00072
5	2	4	4	2	3	9769.53907	9769.53900	0.00007

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
5	2	3	4	2	2	10120.50434	10120.50351	0.00083
5	1	4	4	1	3	10361.76526	10361.76521	0.00005
6	1	6	5	1	5	10874.07081	10874.07189	-0.00108
6	0	6	5	0	5	11200.88130	11200.88106	0.00024
6	2	5	5	2	4	11689.01946	11689.02046	-0.00100
6	3	4	5	3	3	11855.27620	11855.27588	0.00032
6	3	3	5	3	2	11903.07303	11903.07362	-0.00059
7	0	7	6	1	6	12038.93642	12038.93642	0.00000
6	1	6	5	0	5	12065.28694	12065.28724	-0.00030
6	2	4	5	2	3	12260.86289	12260.86342	-0.00053
6	1	5	5	1	4	12368.32261	12368.32327	-0.00066
7	1	7	6	1	6	12637.75027	12637.75056	-0.00029
7	0	7	6	0	6	12903.34218	12903.34259	-0.00041
7	1	7	6	0	6	13502.15695	13502.15673	0.00022
7	1	7	6	0	6	13502.15746	13502.15673	0.00073
7	2	6	6	2	5	13590.29968	13590.29933	0.00035
7	4	4	6	4	3	13828.99471	13828.99599	-0.00128
7	4	3	6	4	2	13832.96771	13832.96625	0.00146
7	3	5	6	3	4	13843.81499	13843.81588	-0.00089
7	3	4	6	3	3	13948.85323	13948.85299	0.00024
8	0	8	7	1	7	13988.02308	13988.02281	0.00027
7	1	6	6	1	5	14331.71632	14331.71649	-0.00017
8	1	8	7	1	7	14387.32212	14387.32263	-0.00051
7	2	5	6	2	4	14419.22097	14419.22140	-0.00043
8	0	8	7	0	7	14586.83623	14586.83695	-0.00072
8	2	7	7	2	6	15471.13315	15471.13330	-0.00015
8	4	5	7	4	4	15827.20066	15827.20055	0.00011
8	3	6	7	3	5	15829.85791	15829.85845	-0.00054
9	0	9	8	1	8	15866.55299	15866.55272	0.00027

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
9	1	9	8	1	8	16124.88710	16124.88658	0.00052
8	1	7	7	1	6	16240.82047	16240.82095	-0.00048
9	0	9	8	0	8	16265.85225	16265.85254	-0.00029
5	2	4	4	1	3	16355.82826	16355.82744	0.00082
9	1	9	8	0	8	16524.18610	16524.18640	-0.00030
8	2	6	7	2	5	16572.03464	16572.03380	0.00084
9	2	8	8	2	7	17329.91910	17329.91883	0.00027
6	2	5	5	1	4	17683.08199	17683.08269	-0.00070
10	0	10	9	1	9	17689.60373	17689.60333	0.00040
9	3	7	8	3	6	17808.98319	17808.98190	0.00129
9	4	6	8	4	5	17832.23224	17832.23237	-0.00013
10	1	10	9	1	9	17852.82701	17852.82605	0.00096
9	4	5	8	4	4	17857.75558	17857.75663	-0.00105
10	0	10	9	0	9	17947.93752	17947.93719	0.00033

Table S18: *anti* 3-fluoroanisole (<sup>13</sup>C3)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
4	0	4	3	0	3	7641.81961	7641.81973	-0.00012
4	1	3	3	1	2	8287.05656	8287.05413	0.00243
5	1	5	4	1	4	9068.09033	9068.09083	-0.00050
4	1	4	3	0	3	9232.72477	9232.72586	-0.00109
5	0	5	4	0	4	9434.00785	9434.00870	-0.00085
5	2	4	4	2	3	9733.18678	9733.18787	-0.00109
5	2	3	4	2	2	10072.68783	10072.68786	-0.00003
5	1	4	4	1	3	10318.84079	10318.84132	-0.00053
5	1	5	4	0	4	10658.99727	10658.99696	0.00031
6	1	6	5	1	5	10843.09499	10843.09567	-0.00068
6	0	6	5	0	5	11172.81382	11172.81444	-0.00062

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
6	2	5	5	2	4	11646.61327	11646.61559	-0.00232
6	3	4	5	3	3	11807.40512	11807.40545	-0.00033
6	3	3	5	3	2	11852.49658	11852.49687	-0.00029
7	0	7	6	1	6	11977.98144	11977.98210	-0.00066
6	1	6	5	0	5	12068.08357	12068.08392	-0.00035
6	2	4	5	2	3	12201.19676	12201.19648	0.00028
6	1	5	5	1	4	12319.45447	12319.45467	-0.00020
7	1	7	6	1	6	12602.92572	12602.92600	-0.00028
7	0	7	6	0	6	12873.25150	12873.25158	-0.00008
7	1	7	6	0	6	13498.19520	13498.19548	-0.00028
7	2	6	6	2	5	13542.45930	13542.45955	-0.00025
7	4	4	6	4	3	13772.75267	13772.75246	0.00021
7	4	3	6	4	2	13776.41096	13776.41059	0.00037
7	3	5	6	3	4	13787.94131	13787.94146	-0.00015
7	3	4	6	3	3	13887.14245	13887.14245	0.00000
8	0	8	7	1	7	13928.87442	13928.87394	0.00048
7	1	6	6	1	5	14278.69964	14278.70123	-0.00159
7	2	5	6	2	4	14348.79045	14348.79093	-0.00048
8	1	8	7	1	7	14348.86398	14348.86436	-0.00038
8	0	8	7	0	7	14553.81936	14553.81784	0.00152
8	4	5	7	4	4	15762.22198	15762.22202	-0.00004
8	3	6	7	3	5	15766.35752	15766.35800	-0.00048
8	4	4	7	4	3	15772.18210	15772.18071	0.00139
9	0	9	8	1	8	15809.04216	15809.04235	-0.00019
8	3	5	7	3	4	15957.78251	15957.78292	-0.00041
9	1	9	8	1	8	16082.89169	16082.89193	-0.00024
8	1	7	7	1	6	16185.81484	16185.81558	-0.00074
9	0	9	8	0	8	16229.03294	16229.03277	0.00017
5	2	4	4	1	3	16410.40565	16410.40430	0.00135

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
8	2	6	7	2	5	16492.72102	16492.72057	0.00045
9	1	9	8	0	8	16502.88146	16502.88235	-0.00089
9	2	8	8	2	7	17273.19368	17273.19334	0.00034
10	0	10	9	1	9	17632.92718	17632.92633	0.00085
6	2	5	5	1	4	17738.17780	17738.17856	-0.00076
9	3	7	8	3	6	17738.42955	17738.42940	0.00015
9	4	6	8	4	5	17758.40499	17758.40461	0.00038
9	4	5	8	4	4	17781.95234	17781.95106	0.00128
10	1	10	9	1	9	17807.29697	17807.29630	0.00067
10	0	10	9	0	9	17906.77764	17906.77591	0.00173

Table S19: *anti* 3-fluoroanisole (<sup>13</sup>C4)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
4	0	4	3	0	3	7626.43629	7626.43575	0.00054
4	1	3	3	1	2	8276.45320	8276.45261	0.00059
5	1	5	4	1	4	9048.76106	9048.76146	-0.00040
5	0	5	4	0	4	9412.98741	9412.98806	-0.00065
5	2	4	4	2	3	9717.24473	9717.24544	-0.00071
5	2	3	4	2	2	10062.59188	10062.59132	0.00056
5	1	4	4	1	3	10304.73456	10304.73399	0.00057
6	1	6	5	1	5	10819.31119	10819.31197	-0.00078
6	0	6	5	0	5	11145.92264	11145.92291	-0.00027
6	2	5	5	2	4	11626.85413	11626.85415	-0.00002
6	3	4	5	3	3	11790.43435	11790.43387	0.00048
6	3	3	5	3	2	11837.03334	11837.03413	-0.00079
7	0	7	6	1	6	11968.58211	11968.58252	-0.00041
6	1	6	5	0	5	12018.17595	12018.17693	-0.00098
6	2	4	5	2	3	12190.07654	12190.07712	-0.00058

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
6	1	5	5	1	4	12301.12342	12301.12463	-0.00121
6	1	5	5	1	4	12301.12506	12301.12463	0.00043
7	1	7	6	1	6	12574.53949	12574.53977	-0.00028
7	0	7	6	0	6	12840.83400	12840.83655	-0.00255
7	1	7	6	0	6	13446.79367	13446.79379	-0.00012
7	2	6	6	2	5	13518.56091	13518.56082	0.00009
7	4	4	6	4	3	13753.20622	13753.20622	0.00000
7	4	3	6	4	2	13757.04210	13757.04355	-0.00145
7	3	5	6	3	4	13768.10955	13768.11017	-0.00062
7	3	4	6	3	3	13870.55712	13870.55867	-0.00155
8	0	8	7	1	7	13910.56507	13910.56436	0.00071
7	1	6	6	1	5	14255.18744	14255.18749	-0.00005
8	1	8	7	1	7	14315.79458	14315.79453	0.00005
7	2	5	6	2	4	14335.89950	14335.90038	-0.00088
8	0	8	7	0	7	14516.52151	14516.52160	-0.00009
8	2	7	7	2	6	15390.14810	15390.14762	0.00048
8	4	5	7	4	4	15740.23647	15740.23622	0.00025
8	3	6	7	3	5	15743.44120	15743.44029	0.00091
8	4	4	7	4	3	15750.67971	15750.67953	0.00018
8	3	5	7	3	4	15940.90646	15940.90721	-0.00075
9	1	9	8	1	8	16045.12341	16045.12313	0.00028
8	1	7	7	1	6	16155.97360	16155.97330	0.00030
9	0	9	8	0	8	16187.42609	16187.42588	0.00021
5	2	4	4	1	3	16310.92982	16310.92977	0.00005
9	1	9	8	0	8	16450.35403	16450.35330	0.00073
8	2	6	7	2	5	16476.89926	16476.89884	0.00042
9	2	8	8	2	7	17240.01749	17240.01613	0.00136
10	0 1	0	9	1	9	17598.26515	17598.26427	0.00088
6	2	5	5	1	4	17633.05007	17633.04993	0.00014



J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
9	3	7	8	3	6	17712.09280	17712.09241	0.00039
9	4	6	8	4	5	17734.02578	17734.02545	0.00033
9	4	5	8	4	4	17758.70756	17758.70639	0.00117
10	1 1	0	9	1	9	17764.86469	17764.86455	0.00014
10	0 1	0	9	0	9	17861.19164	17861.19169	-0.00005
9	1	8	8	1	7	17994.59505	17994.59453	0.00052

Table S20: *anti* 3-fluoroanisole (<sup>13</sup>C5)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
4	0	4	3	0	3	7641.22515	7641.22494	0.00021
4	1	3	3	1	2	8311.26918	8311.26939	-0.00021
5	1	5	4	1	4	9063.31845	9063.31857	-0.00012
5	0	5	4	0	4	9424.98225	9424.98145	0.00080
5	2	4	4	2	3	9747.53877	9747.53994	-0.00117
5	2	3	4	2	2	10113.93785	10113.93972	-0.00187
5	1	4	4	1	3	10345.20452	10345.20550	-0.00098
6	1	6	5	1	5	10834.63669	10834.63675	-0.00006
6	0	6	5	0	5	11154.10310	11154.10355	-0.00045
6	2	5	5	2	4	11660.94562	11660.94639	-0.00077
6	3	4	5	3	3	11834.59100	11834.59146	-0.00046
6	3	3	5	3	2	11886.46558	11886.46567	-0.00009
6	1	6	5	0	5	11965.63165	11965.63099	0.00066
7	0	7	6	1	6	12034.58356	12034.58376	-0.00020
6	2	4	5	2	3	12255.50498	12255.50533	-0.00035
6	1	5	5	1	4	12344.70714	12344.70743	-0.00029
7	1	7	6	1	6	12590.06935	12590.06514	0.00421
7	0	7	6	0	6	12846.11013	12846.11120	-0.00107
7	1	7	6	0	6	13401.59228	13401.59259	-0.00031

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
7	2	6	6	2	5	13555.30790	13555.30772	0.00018
7	4	4	6	4	3	13805.56470	13805.56417	0.00053
7	4	3	6	4	2	13810.03272	13810.03293	-0.00021
7	3	4	6	3	3	13933.36761	13933.36589	0.00172
8	0	8	7	1	7	13965.27717	13965.27816	-0.00099
7	1	6	6	1	5	14298.48711	14298.48610	0.00101
8	1	8	7	1	7	14331.17914	14331.17838	0.00076
7	2	5	6	2	4	14413.06789	14413.06728	0.00061
8	0	8	7	0	7	14520.75911	14520.75955	-0.00044
8	2	7	7	2	6	15428.33520	15428.33608	-0.00088
8	3	6	7	3	5	15801.46420	15801.46235	0.00185
8	4	4	7	4	3	15813.49563	15813.49604	-0.00041
9	0	9	8	1	8	15826.39192	15826.39209	-0.00017
9	1	9	8	1	8	16060.24319	16060.24414	-0.00095
9	0	9	8	0	8	16192.29176	16192.29231	-0.00055
8	1	7	7	1	6	16194.96668	16194.96697	-0.00029
9	1	9	8	0	8	16426.14382	16426.14436	-0.00054
8	2	6	7	2	5	16562.08684	16562.08635	0.00049
9	2	8	8	2	7	17278.45203	17278.45244	-0.00041
10	0	10	9	1	9	17633.79831	17633.79758	0.00073
9	3	7	8	3	6	17775.53840	17775.53951	-0.00111
10	1	10	9	1	9	17779.77592	17779.77541	0.00051
9	4	6	8	4	5	17804.06449	17804.06415	0.00034
9	4	5	8	4	4	17832.73573	17832.73550	0.00023
10	0	10	9	0	9	17867.64938	17867.64964	-0.00026

Table S21: *anti* 3-fluoroanisole (<sup>13</sup>C6)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
4	0	4	3	0	3	7653.76492	7653.76453	0.00039
4	1	3	3	1	2	8312.05907	8312.05915	-0.00008
5	1	5	4	1	4	9080.20905	9080.21054	-0.00149
5	0	5	4	0	4	9444.72768	9444.72795	-0.00027
5	2	4	4	2	3	9755.67929	9755.67987	-0.00058
5	2	3	4	2	2	10108.70978	10108.70928	0.00050
5	1	4	4	1	3	10348.16421	10348.16399	0.00022
6	1	6	5	1	5	10856.25380	10856.25483	-0.00103
6	0	6	5	0	5	11181.57064	11181.57043	0.00021
6	2	5	5	2	4	11672.16221	11672.16276	-0.00055
6	3	3	5	3	2	11887.78391	11887.78449	-0.00058
7	0	7	6	1	6	12025.63590	12025.63631	-0.00041
6	1	6	5	0	5	12036.47957	12036.48121	-0.00164
6	2	4	5	2	3	12247.00048	12247.00092	-0.00044
6	1	5	5	1	4	12351.48615	12351.48628	-0.00013
6	1	5	5	1	4	12351.48775	12351.48628	0.00147
7	1	7	6	1	6	12616.74746	12616.74862	-0.00116
7	0	7	6	0	6	12880.54656	12880.54709	-0.00053
7	1	7	6	0	6	13471.65959	13471.65940	0.00019
7	2	6	6	2	5	13570.32912	13570.32962	-0.00050
7	4	4	6	4	3	13810.58958	13810.59011	-0.00053
7	3	5	6	3	4	13825.27550	13825.27572	-0.00022
7	3	4	6	3	3	13931.55677	13931.55714	-0.00037
8	0	8	7	1	7	13969.71615	13969.71648	-0.00033
7	1	6	6	1	5	14311.28745	14311.28915	-0.00170
8	1	8	7	1	7	14363.11583	14363.11612	-0.00029
7	2	5	6	2	4	14402.96648	14402.96623	0.00025
8	0	8	7	0	7	14560.82720	14560.82879	-0.00159
8	2	7	7	2	6	15447.93253	15447.93289	-0.00036

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
8	4	5	7	4	4	15806.28818	15806.28798	0.00020
8	3	6	7	3	5	15808.55695	15808.55606	0.00089
8	4	4	7	4	3	15817.28604	15817.28469	0.00135
9	0	9	8	1	8	15843.45624	15843.45680	-0.00056
8	3	5	7	3	4	16013.17656	16013.17733	-0.00077
9	1	9	8	1	8	16097.48052	16097.48034	0.00018
8	1	7	7	1	6	16216.38659	16216.38667	-0.00008
9	0	9	8	0	8	16236.85788	16236.85644	0.00144
5	2	4	4	1	3	16304.50566	16304.50640	-0.00074
9	1	9	8	0	8	16490.88145	16490.87997	0.00148
8	2	6	7	2	5	16552.92268	16552.92295	-0.00027
9	2	8	8	2	7	17303.37303	17303.37386	-0.00083
6	2	5	5	1	4	17628.50615	17628.50517	0.00098
10	0 1	0	9	1	9	17662.05364	17662.05194	0.00170
9	3	7	8	3	6	17784.78777	17784.78714	0.00063
9	4	6	8	4	5	17808.82498	17808.82457	0.00041
10	1 1	0	9	1	9	17822.24352	17822.24318	0.00034
9	4	5	8	4	4	17834.80293	17834.80137	0.00156
10	0 1	0	9	0	9	17916.07613	17916.07548	0.00065

Table S22: *anti* 3-fluoroanisole (<sup>13</sup>C7)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
4	0	4	3	0	3	7533.07902	7533.07895	0.00007
4	1	3	3	1	2	8154.34588	8154.34900	-0.00312
5	1	5	4	1	4	8941.76219	8941.76367	-0.00148
5	0	5	4	0	4	9304.72566	9304.72597	-0.00031
5	2	4	4	2	3	9585.86466	9585.86559	-0.00093
5	2	3	4	2	2	9904.70740	9904.70825	-0.00085

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
5	1	4	4	1	3	10155.76881	10155.76901	-0.00020
6	1	6	5	1	5	10693.67350	10693.67406	-0.00056
6	0	6	5	0	5	11024.66811	11024.66859	-0.00048
6	2	5	5	2	4	11471.97989	11471.98093	-0.00104
6	3	4	5	3	3	11622.95156	11622.95249	-0.00093
6	3	3	5	3	2	11663.63414	11663.63490	-0.00076
7	0	7	6	1	6	11768.81524	11768.81610	-0.00086
6	1	6	5	0	5	11962.06529	11962.06643	-0.00114
6	2	4	5	2	3	11994.88517	11994.88605	-0.00088
6	1	5	5	1	4	12128.32067	12128.32076	-0.00009
7	1	7	6	1	6	12431.07048	12431.07091	-0.00043
7	0	7	6	0	6	12706.21322	12706.21394	-0.00072
7	2	6	6	2	5	13341.61675	13341.61740	-0.00065
7	1	7	6	0	6	13368.46807	13368.46875	-0.00068
7	4	4	6	4	3	13557.02990	13557.02978	0.00012
7	4	3	6	4	2	13560.20715	13560.20772	-0.00057
7	3	5	6	3	4	13572.54843	13572.54922	-0.00079
7	3	4	6	3	3	13662.19955	13662.20144	-0.00189
8	0	8	7	1	7	13704.46511	13704.46531	-0.00020
7	1	6	6	1	5	14062.59431	14062.59406	0.00025
7	2	5	6	2	4	14105.50433	14105.50510	-0.00077
8	1	8	7	1	7	14155.05224	14155.05211	0.00013
8	0	8	7	0	7	14366.71965	14366.72013	-0.00048
8	2	7	7	2	6	15192.66654	15192.66697	-0.00043
8	4	5	7	4	4	15514.40220	15514.40167	0.00053
8	3	6	7	3	5	15520.59590	15520.59615	-0.00025
8	4	4	7	4	3	15523.05935	15523.05947	-0.00012
9	0	9	8	1	8	15569.95082	15569.95042	0.00040
8	3	5	7	3	4	15694.06740	15694.06820	-0.00080

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
9	1	9	8	1	8	15867.40113	15867.40119	-0.00006
8	1	7	7	1	6	15948.49944	15948.49600	0.00344
9	0	9	8	0	8	16020.53847	16020.53723	0.00124
8	2	6	7	2	5	16215.31039	16215.30993	0.00046
9	1	9	8	0	8	16317.98772	16317.98799	-0.00027
5	2	4	4	1	3	16347.82050	16347.82040	0.00010
9	2	8	8	2	7	17023.54552	17023.54431	0.00121
10	0	10	9	1	9	17378.50231	17378.50171	0.00060
9	3	7	8	3	6	17463.20729	17463.20627	0.00102
9	4	6	8	4	5	17478.23471	17478.23283	0.00188
9	4	5	8	4	4	17498.72747	17498.72611	0.00136
10	1	10	9	1	9	17570.23376	17570.23376	0.00000
6	2	5	5	1	4	17664.03228	17664.03232	-0.00004
10	0	10	9	0	9	17675.95385	17675.95247	0.00138
9	3	6	8	3	5	17765.73106	17765.73002	0.00104
9	1	8	8	1	7	17777.24970	17777.24895	0.00075

Table S23: *anti* 3-fluoroanisole (<sup>18</sup>O)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
4	0	4	3	0	3	7551.85618	7551.85799	-0.00181
4	1	3	3	1	2	8188.46166	8188.46311	-0.00145
5	1	5	4	1	4	8961.46592	8961.46704	-0.00112
4	1	4	3	0	3	9128.94262	9128.94233	0.00029
5	0	5	4	0	4	9323.30693	9323.30907	-0.00214
5	1	4	4	1	3	10196.24056	10196.24029	0.00027
5	1	5	4	0	4	10538.55090	10538.55138	-0.00048
6	1	6	5	1	5	10715.71908	10715.71981	-0.00073
6	0	6	5	0	5	11042.06372	11042.06311	0.00061

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
6	2	5	5	2	4	11508.85160	11508.85160	0.00000
7	0	7	6	1	6	11833.94707	11833.94713	-0.00006
6	1	6	5	0	5	11930.96184	11930.96212	-0.00028
6	2	4	5	2	3	12055.16998	12055.17038	-0.00040
6	1	5	5	1	4	12173.34807	12173.35008	-0.00201
7	1	7	6	1	6	12455.00655	12455.00791	-0.00136
7	0	7	6	0	6	12722.84645	12722.84614	0.00031
7	1	7	6	0	6	13343.90806	13343.90693	0.00113
7	2	6	6	2	5	13382.43463	13382.43422	0.00041
7	1	6	6	1	5	14109.76691	14109.76706	-0.00015
7	2	5	6	2	4	14177.03829	14177.03824	0.00005
8	1	8	7	1	7	14180.58642	14180.58608	0.00034
8	0	8	7	0	7	14383.87718	14383.87732	-0.00014
8	2	7	7	2	6	15236.53287	15236.53387	-0.00100
9	1	9	8	1	8	15894.39966	15894.39951	0.00015
8	1	7	7	1	6	15994.88935	15994.88974	-0.00039
9	0	9	8	0	8	16039.51437	16039.51370	0.00067
8	2	6	7	2	5	16295.50328	16295.50016	0.00312
9	2	8	8	2	7	17069.56429	17069.56328	0.00101
10	1	10	9	1	9	17598.69885	17598.69868	0.00017
10	0	10	9	0	9	17697.58510	17697.58406	0.00104
9	1	8	8	1	7	17819.89392	17819.89396	-0.00004

Table S24: *syn* 3-fluoroanisole (parent)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
6	1	5	6	1	6	7764.53693	7764.54086	-0.00393
4	1	4	3	1	3	7767.01561	7767.01585	-0.00024
4	2	3	4	0	4	7787.70036	7787.70056	-0.00020

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
4	0	4	3	0	3	8093.99895	8093.99897	-0.00002
11	3	8	11	3	9	8207.57611	8207.56677	0.00934
4	1	4	3	0	3	8599.13776	8599.13824	-0.00048
4	2	3	3	2	2	8620.75148	8620.75167	-0.00019
5	2	4	5	0	5	8628.02617	8628.02719	-0.00102
4	3	2	3	3	1	8788.34783	8788.34755	0.00028
4	3	1	3	3	0	8830.82107	8830.82073	0.00034
4	2	2	3	2	1	9199.34913	9199.35027	-0.00114
4	1	3	3	1	2	9306.79380	9306.79456	-0.00076
5	0	5	4	1	4	9347.53331	9347.53396	-0.00065
9	2	7	9	2	8	9420.09401	9420.09293	0.00108
5	1	5	4	1	4	9624.19417	9624.19389	0.00028
6	2	5	6	0	6	9755.96062	9755.96199	-0.00137
7	1	6	7	1	7	9846.52184	9846.52524	-0.00340
5	0	5	4	0	4	9852.67353	9852.67324	0.00029
5	1	5	4	0	4	10129.33513	10129.33316	0.00197
5	2	4	4	2	3	10692.99958	10692.99987	-0.00029
12	3	9	12	3	10	10729.67725	10729.66654	0.01071
5	4	2	4	4	1	10990.10249	10990.10280	-0.00031
5	4	1	4	4	0	10995.18517	10995.18529	-0.00012
5	3	3	4	3	2	11006.37245	11006.37296	-0.00051
7	2	6	7	0	7	11110.22238	11110.22412	-0.00174
3	2	2	2	1	1	11114.86647	11114.86416	0.00231
5	3	2	4	3	1	11148.75933	11148.76044	-0.00111
6	0	6	5	1	5	11309.59068	11309.59052	0.00016
2	2	0	1	0	1	11341.33868	11341.33999	-0.00131
6	1	6	5	1	5	11450.29577	11450.29575	0.00002
5	1	4	4	1	3	11459.56230	11459.56277	-0.00047
6	3	4	6	1	5	11541.60881	11541.60723	0.00158



J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
6	0	6	5	0	5	11586.25084	11586.25044	0.00040
7	3	5	7	1	6	11597.72464	11597.72377	0.00087
5	2	3	4	2	2	11676.78466	11676.78588	-0.00122
6	1	6	5	0	5	11726.95573	11726.95567	0.00006
10	2	8	10	2	9	11745.85570	11745.85278	0.00292
5	3	3	5	1	4	11801.98884	11801.98824	0.00060
8	1	7	8	1	8	11885.94979	11885.95336	-0.00357
8	3	6	8	1	7	12042.81432	12042.81379	0.00053
4	3	2	4	1	3	12255.17962	12255.17805	0.00157
8	2	7	8	0	8	12625.65626	12625.65848	-0.00222
4	2	3	3	1	2	12683.41374	12683.40995	0.00379
6	2	5	5	2	4	12714.18491	12714.18524	-0.00033
9	3	7	9	1	8	12870.83463	12870.83418	0.00045
6	5	2	5	5	1	13179.43458	13179.43309	0.00149
6	5	1	5	5	0	13179.94512	13179.94594	-0.00082
7	0	7	6	1	6	13185.90406	13185.90372	0.00034
6	3	4	5	3	3	13213.14023	13213.14082	-0.00059
6	4	3	5	4	2	13230.83753	13230.83829	-0.00076
6	4	3	5	4	2	13230.83764	13230.83829	-0.00065
6	4	2	5	4	1	13253.18921	13253.18994	-0.00073
7	1	7	6	1	6	13253.88970	13253.88964	0.00006
7	0	7	6	0	6	13326.60904	13326.60896	0.00008
7	1	7	6	0	6	13394.59516	13394.59487	0.00029
6	1	5	5	1	4	13473.52202	13473.52183	0.00019
7	1	6	6	2	5	13485.15675	13485.15811	-0.00136
6	3	3	5	3	2	13562.76105	13562.76182	-0.00077
3	2	1	2	0	2	13832.89697	13832.89682	0.00015
9	1	8	9	1	9	13842.50643	13842.50790	-0.00147
11	2	9	11	2	10	14007.98141	14007.97673	0.00468

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
10	3	8	10	1	9	14018.24215	14018.24071	0.00144
5	2	4	4	1	3	14069.61693	14069.61526	0.00167
6	2	4	5	2	3	14115.41522	14115.41567	-0.00045
9	2	8	9	0	9	14247.19341	14247.19464	-0.00123
7	2	6	6	2	5	14680.87110	14680.87108	0.00002
8	0	8	7	1	7	15011.40452	15011.40596	-0.00144
8	1	8	7	1	7	15043.08549	15043.08512	0.00037
8	0	8	7	0	7	15079.39217	15079.39188	0.00029
8	1	8	7	0	7	15111.06974	15111.07103	-0.00129
6	2	5	5	1	4	15324.24105	15324.23773	0.00332
7	1	6	6	1	5	15335.87469	15335.87402	0.00067
7	6	2	6	6	1	15368.28954	15368.28882	0.00072
7	6	1	6	6	0	15368.33221	15368.33537	-0.00316
7	3	5	6	3	4	15391.99052	15391.99056	-0.00004
10	4	7	10	2	8	15400.11071	15400.11292	-0.00221
11	3	9	11	1	10	15403.17226	15403.16979	0.00247
7	5	3	6	5	2	15418.28904	15418.28923	-0.00019
7	5	2	6	5	1	15421.06540	15421.06566	-0.00026
11	4	8	11	2	9	15442.35556	15442.35656	-0.00100
7	4	4	6	4	3	15485.28626	15485.28646	-0.00020
7	4	3	6	4	2	15556.92295	15556.92334	-0.00039
10	1	9	10	1	10	15723.38251	15723.38383	-0.00132
9	4	6	9	2	7	15799.05570	15799.05700	-0.00130
8	1	7	7	2	6	15886.80057	15886.80028	0.00029
10	2	9	10	0	10	15933.57990	15933.58147	-0.00157
12	4	9	12	2	10	15946.75978	15946.75808	0.00170
7	3	4	6	3	3	16076.13570	16076.13580	-0.00010
12	2	10	12	2	11	16146.51966	16146.51223	0.00743
7	2	5	6	2	4	16460.70270	16460.70237	0.00033

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
7	2	6	6	1	5	16531.58661	16531.58698	-0.00037
8	4	5	8	2	6	16537.53403	16537.53537	-0.00134
8	2	7	7	2	6	16594.82653	16594.82624	0.00029
4	2	2	3	0	3	16783.54215	16783.54306	-0.00091
9	0	9	8	1	8	16809.60341	16809.60364	-0.00023
9	1	9	8	1	8	16823.97443	16823.97437	0.00006
9	0	9	8	0	8	16841.28287	16841.28279	0.00008
9	1	9	8	0	8	16855.65441	16855.65352	0.00089
13	4	10	13	2	11	16859.19935	16859.19727	0.00208
12	3	10	12	1	11	16950.59104	16950.59002	0.00102
8	1	7	7	1	6	17082.51388	17082.51324	0.00064
4	3	2	3	2	1	17176.07002	17176.06940	0.00062
7	4	4	7	2	5	17469.50499	17469.50599	-0.00100
8	3	6	7	3	5	17527.60375	17527.60327	0.00048
11	1	10	11	1	11	17551.73118	17551.73051	0.00067
8	7	2	7	7	1	17557.70799	17557.70654	0.00145
8	7	1	7	7	0	17557.70799	17557.71047	-0.00248
8	6	3	7	6	2	17602.68814	17602.68788	0.00026
8	6	2	7	6	1	17602.98611	17602.98678	-0.00067
11	2	10	11	0	11	17656.71706	17656.71659	0.00047
8	5	4	7	5	3	17675.12035	17675.11994	0.00041
8	5	3	7	5	2	17685.95604	17685.95570	0.00034
8	4	5	7	4	4	17744.80858	17744.80798	0.00060
8	2	7	7	1	6	17790.53948	17790.53920	0.00028
8	4	4	7	4	3	17929.56759	17929.56706	0.00053

Table S25: *syn* 3-fluoroanisole (<sup>13</sup>C1)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
3	1	2	2	1	1	7039.06306	7039.06355	-0.00049
4	1	4	3	1	3	7754.40346	7754.40526	-0.00180
4	0	4	3	0	3	8081.46796	8081.46772	0.00024
4	2	3	3	2	2	8605.48636	8605.48689	-0.00053
4	3	2	3	3	1	8772.11782	8772.12074	-0.00292
4	3	1	3	3	0	8814.21014	8814.20789	0.00225
4	2	2	3	2	1	9181.04183	9181.04109	0.00074
4	1	3	3	1	2	9289.90955	9289.90994	-0.00039
5	1	5	4	1	4	9608.83699	9608.83702	-0.00003
5	0	5	4	0	4	9837.80910	9837.80944	-0.00034
5	2	4	4	2	3	10674.41339	10674.41409	-0.00070
5	4	2	4	4	1	10969.72914	10969.72936	-0.00022
5	4	1	4	4	0	10974.75423	10974.74938	0.00485
5	3	3	4	3	2	10986.07113	10986.07188	-0.00075
5	3	2	4	3	1	11127.20450	11127.20599	-0.00149
6	1	6	5	1	5	11432.27540	11432.27615	-0.00075
5	1	4	4	1	3	11439.63434	11439.63531	-0.00097
6	0	6	5	0	5	11568.79266	11568.79305	-0.00039
5	2	3	4	2	2	11653.64755	11653.64706	0.00049
6	2	5	5	2	4	12692.55807	12692.55834	-0.00027
6	3	4	5	3	3	13188.93877	13188.93942	-0.00065
6	4	3	5	4	2	13206.17108	13206.17090	0.00018
7	1	7	6	1	6	13233.23023	13233.23036	-0.00013
7	0	7	6	0	6	13306.38833	13306.38834	-0.00001
6	1	5	5	1	4	13451.40598	13451.40619	-0.00021
6	3	3	5	3	2	13535.67379	13535.67510	-0.00131
6	2	4	5	2	3	14088.14213	14088.14273	-0.00060
7	2	6	6	2	5	14656.46356	14656.46382	-0.00026
8	1	8	7	1	7	15019.77389	15019.77402	-0.00013

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
8	0	8	7	0	7	15056.36619	15056.36549	0.00070
7	1	6	6	1	5	15312.15670	15312.15674	-0.00004
7	3	5	6	3	4	15364.16877	15364.16829	0.00048
7	5	3	6	5	2	15389.55876	15389.55912	-0.00036
7	4	4	6	4	3	15456.31405	15456.31383	0.00022
7	4	3	6	4	2	15527.09976	15527.09989	-0.00013
7	3	4	6	3	3	16043.26157	16043.26060	0.00097
7	2	5	6	2	4	16430.09701	16430.09708	-0.00007
8	2	7	7	2	6	16567.83506	16567.83496	0.00010
9	1	9	8	1	8	16797.98861	16797.98795	0.00066
9	0	9	8	0	8	16815.46241	16815.46240	0.00001
8	1	7	7	1	6	17057.08279	17057.08153	0.00126
8	3	6	7	3	5	17496.50611	17496.50604	0.00007
8	5	4	7	5	3	17641.97902	17641.97892	0.00010
8	5	3	7	5	2	17652.65022	17652.65011	0.00011
8	4	4	7	4	3	17894.27464	17894.27433	0.00031

Table S26: *syn* 3-fluoroanisole (<sup>13</sup>C2)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
4	1	4	3	1	3	7760.81397	7760.81325	0.00072
4	0	4	3	0	3	8086.08669	8086.08614	0.00055
4	2	3	3	2	2	8616.93363	8616.93314	0.00049
4	3	2	3	3	1	8786.05652	8786.05655	-0.00003
4	3	1	3	3	0	8829.26369	8829.26243	0.00126
4	2	2	3	2	1	9200.13085	9200.13118	-0.00033
4	1	3	3	1	2	9303.65655	9303.65761	-0.00106
5	1	5	4	1	4	9615.86215	9615.86129	0.00086
5	0	5	4	0	4	9842.10782	9842.10921	-0.00139
5	2	4	4	2	3	10687.42414	10687.42463	-0.00049

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
5	4	1	4	4	0	10992.63805	10992.64527	-0.00722
5	3	3	4	3	2	11003.45168	11003.45161	0.00007
5	3	2	4	3	1	11148.19474	11148.19488	-0.00014
6	1	6	5	1	5	11439.77833	11439.77886	-0.00053
5	1	4	4	1	3	11453.62042	11453.62093	-0.00051
6	0	6	5	0	5	11573.77296	11573.77416	-0.00120
5	2	3	4	2	2	11677.52531	11677.52579	-0.00048
6	2	5	5	2	4	12706.42056	12706.42036	0.00020
6	3	4	5	3	3	13209.22259	13209.22244	0.00015
6	4	3	5	4	2	13227.96417	13227.96367	0.00050
7	1	7	6	1	6	13241.23830	13241.23869	-0.00039
6	4	2	5	4	1	13250.86894	13250.86859	0.00035
7	0	7	6	0	6	13312.58782	13312.58809	-0.00027
6	1	5	5	1	4	13463.37554	13463.37546	0.00008
6	3	3	5	3	2	13564.15408	13564.15435	-0.00027
6	2	4	5	2	3	14114.62877	14114.62849	0.00028
7	2	6	6	2	5	14670.54579	14670.54659	-0.00080
8	1	8	7	1	7	15028.39676	15028.39603	0.00073
8	0	8	7	0	7	15063.86746	15063.86647	0.00099
7	1	6	6	1	5	15320.84235	15320.84245	-0.00010
7	3	5	6	3	4	15386.53400	15386.53353	0.00047
7	5	3	6	5	2	15414.90505	15414.90436	0.00069
7	5	2	6	5	1	15417.77290	15417.77165	0.00125
7	4	4	6	4	3	15482.16618	15482.16606	0.00012
7	4	3	6	4	2	15555.52870	15555.52882	-0.00012
7	3	4	6	3	3	16079.61664	16079.61720	-0.00056
7	2	5	6	2	4	16456.90295	16456.90201	0.00094
8	2	7	7	2	6	16581.72027	16581.71977	0.00050
9	1	9	8	1	8	16807.34095	16807.34126	-0.00031

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
8	1	7	7	1	6	17063.42948	17063.42915	0.00033
8	3	6	7	3	5	17519.97981	17519.97930	0.00051
8	5	4	7	5	3	17671.73489	17671.73546	-0.00057
8	5	3	7	5	2	17682.92186	17682.92146	0.00040
8	4	5	7	4	4	17741.18739	17741.18641	0.00098
8	4	4	7	4	3	17930.18721	17930.18647	0.00074

Table S27: *syn* 3-fluoroanisole (<sup>13</sup>C3)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
3	1	2	2	1	1	7022.37412	7022.37487	-0.00075
4	1	4	3	1	3	7738.15931	7738.16106	-0.00175
4	0	4	3	0	3	8065.24144	8065.24214	-0.00070
4	2	3	3	2	2	8586.00199	8586.00383	-0.00184
4	3	2	3	3	1	8751.49730	8751.49637	0.00093
4	3	1	3	3	0	8793.13282	8793.13235	0.00047
4	2	2	3	2	1	9157.93237	9157.93221	0.00016
4	1	3	3	1	2	9268.41081	9268.41154	-0.00073
5	1	5	4	1	4	9589.01763	9589.01763	0.00000
5	0	5	4	0	4	9818.50842	9818.50931	-0.00089
5	2	4	4	2	3	10650.64567	10650.64682	-0.00115
5	4	2	4	4	1	10943.84572	10943.84507	0.00065
5	4	1	4	4	0	10948.79357	10948.79270	0.00087
5	3	3	4	3	2	10960.26533	10960.26560	-0.00027
5	3	2	4	3	1	11099.93291	11099.93306	-0.00015
6	1	6	5	1	5	11408.98559	11408.98496	0.00063
5	1	4	4	1	3	11414.15145	11414.15177	-0.00032
6	0	6	5	0	5	11546.12381	11546.12340	0.00041
5	2	3	4	2	2	11624.42554	11624.42652	-0.00098

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
6	2	5	5	2	4	12664.84023	12664.83963	0.00060
6	3	4	5	3	3	13158.15246	13158.15261	-0.00015
6	4	3	5	4	2	13174.84768	13174.84793	-0.00025
6	4	2	5	4	1	13196.61252	13196.61355	-0.00103
7	1	7	6	1	6	13206.49902	13206.49929	-0.00027
7	0	7	6	0	6	13280.15040	13280.15085	-0.00045
6	1	5	5	1	4	13422.95096	13422.95066	0.00030
6	3	3	5	3	2	13501.50304	13501.50369	-0.00065
6	2	4	5	2	3	14053.61772	14053.61745	0.00027
7	2	6	6	2	5	14625.10634	14625.10581	0.00053
8	1	8	7	1	7	14989.59285	14989.59254	0.00031
8	0	8	7	0	7	15026.50758	15026.50748	0.00010
7	1	6	6	1	5	15281.44316	15281.44278	0.00038
7	3	5	6	3	4	15328.72794	15328.72738	0.00056
7	5	3	6	5	2	15353.07611	15353.07570	0.00041
7	5	2	6	5	1	15355.76049	15355.76043	0.00006
7	4	4	6	4	3	15419.53582	15419.53522	0.00060
7	4	3	6	4	2	15489.33310	15489.33410	-0.00100
7	3	4	6	3	3	16001.86873	16001.86728	0.00145
7	2	5	6	2	4	16391.20931	16391.20863	0.00068
8	2	7	7	2	6	16533.07600	16533.07586	0.00014
9	1	9	8	1	8	16764.33151	16764.33094	0.00057
9	0	9	8	0	8	16781.99541	16781.99526	0.00015
8	1	7	7	1	6	17024.01332	17024.01324	0.00008
8	3	6	7	3	5	17456.81770	17456.81769	0.00001
8	5	4	7	5	3	17599.91689	17599.91880	-0.00191
8	5	3	7	5	2	17610.39980	17610.40035	-0.00055
8	4	5	7	4	4	17669.49878	17669.49765	0.00113
8	4	4	7	4	3	17849.69550	17849.69488	0.00062



Table S28: *syn* 3-fluoroanisole (<sup>13</sup>C4)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
3	1	2	2	1	1	6992.87961	6992.87980	-0.00019
4	1	4	3	1	3	7709.23219	7709.23335	-0.00116
4	0	4	3	0	3	8036.25822	8036.25840	-0.00018
4	2	3	3	2	2	8551.47868	8551.47747	0.00121
4	3	2	3	3	1	8715.03923	8715.03536	0.00387
4	3	1	3	3	0	8755.92139	8755.91608	0.00531
4	2	2	3	2	1	9117.23987	9117.23967	0.00020
4	1	3	3	1	2	9230.35496	9230.35570	-0.00074
5	1	5	4	1	4	9553.68559	9553.68658	-0.00099
5	0	5	4	0	4	9783.98777	9783.98697	0.00080
5	2	4	4	2	3	10608.48193	10608.48198	-0.00005
5	4	2	4	4	1	10898.10000	10898.09689	0.00311
5	4	1	4	4	0	10902.92672	10902.92436	0.00236
5	3	3	4	3	2	10914.63999	10914.63899	0.00100
5	3	2	4	3	1	11051.84801	11051.84837	-0.00036
6	1	6	5	1	5	11367.43099	11367.43137	-0.00038
5	1	4	4	1	3	11368.92499	11368.92609	-0.00110
6	0	6	5	0	5	11505.57915	11505.57830	0.00085
5	2	3	4	2	2	11572.94785	11572.94767	0.00018
6	2	5	5	2	4	12615.60043	12615.60155	-0.00112
6	3	4	5	3	3	13103.69425	13103.69527	-0.00102
6	4	3	5	4	2	13119.50399	13119.50423	-0.00024
6	4	2	5	4	1	13140.74653	13140.74733	-0.00080
7	1	7	6	1	6	13158.78247	13158.78289	-0.00042
7	0	7	6	0	6	13233.24580	13233.24741	-0.00161
6	1	5	5	1	4	13372.27254	13372.27302	-0.00048
6	3	3	5	3	2	13441.35906	13441.36037	-0.00131
6	2	4	5	2	3	13992.69891	13992.69932	-0.00041
7	2	6	6	2	5	14569.32687	14569.32743	-0.00056

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
8	1	8	7	1	7	14935.69966	14935.69991	-0.00025
8	0	8	7	0	7	14973.15236	14973.15225	0.00011
7	1	6	6	1	5	15226.55046	15226.55063	-0.00017
7	3	5	6	3	4	15265.98631	15265.98630	0.00001
7	4	4	6	4	3	15354.56198	15354.56234	-0.00036
7	4	3	6	4	2	15422.71957	15422.72030	-0.00073
7	3	4	6	3	3	15929.08650	15929.08697	-0.00047
7	2	5	6	2	4	16322.43691	16322.43712	-0.00021
8	2	7	7	2	6	16471.16891	16471.16830	0.00061
9	1	9	8	1	8	16704.22291	16704.22236	0.00055
9	0	9	8	0	8	16722.20452	16722.20409	0.00043
8	1	7	7	1	6	16964.79753	16964.79703	0.00050
8	3	6	7	3	5	17386.47898	17386.47788	0.00110
8	5	4	7	5	3	17525.62832	17525.62895	-0.00063
8	5	3	7	5	2	17535.79570	17535.79766	-0.00196
8	4	5	7	4	4	17595.06700	17595.06791	-0.00091
8	4	4	7	4	3	17771.18386	17771.18319	0.00067

Table S29: *syn* 3-fluoroanisole (<sup>13</sup>C5)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
3	1	2	2	1	1	7025.64674	7025.64745	-0.00071
4	1	4	3	1	3	7716.14031	7716.14009	0.00022
4	0	4	3	0	3	8033.97741	8033.97851	-0.00110
4	2	3	3	2	2	8578.99926	8579.00201	-0.00275
4	3	2	3	3	1	8753.54787	8753.54562	0.00225
4	3	1	3	3	0	8799.51464	8799.51096	0.00368
4	2	2	3	2	1	9178.18356	9178.18234	0.00122
4	1	3	3	1	2	9266.34524	9266.34559	-0.00035
5	1	5	4	1	4	9558.04639	9558.04726	-0.00087

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
5	0	5	4	0	4	9775.28725	9775.28670	0.00055
5	2	4	4	2	3	10637.14520	10637.14518	0.00002
5	4	2	4	4	1	10947.56144	10947.55979	0.00165
5	4	1	4	4	0	10953.26220	10953.26683	-0.00463
5	3	3	4	3	2	10962.49839	10962.49872	-0.00033
5	3	2	4	3	1	11116.06518	11116.06625	-0.00107
6	1	6	5	1	5	11368.72003	11368.72143	-0.00140
5	1	4	4	1	3	11399.62633	11399.62651	-0.00018
6	0	6	5	0	5	11495.09470	11495.09482	-0.00012
5	2	3	4	2	2	11648.49393	11648.49462	-0.00069
6	2	5	5	2	4	12642.27730	12642.27638	0.00092
6	5	2	5	5	1	13128.17201	13128.17297	-0.00096
6	5	1	5	5	0	13128.76795	13128.77024	-0.00229
7	1	7	6	1	6	13157.20592	13157.20605	-0.00013
6	3	4	5	3	3	13158.42031	13158.42042	-0.00011
6	4	3	5	4	2	13181.23606	13181.23558	0.00048
6	4	2	5	4	1	13206.28784	13206.28897	-0.00113
7	0	7	6	0	6	13223.35364	13223.35360	0.00004
6	1	5	5	1	4	13387.75755	13387.75761	-0.00006
6	3	3	5	3	2	13533.02566	13533.02614	-0.00048
6	2	4	5	2	3	14072.92262	14072.92188	0.00074
7	2	6	6	2	5	14591.29062	14591.29146	-0.00084
8	1	8	7	1	7	14931.79832	14931.79823	0.00009
8	0	8	7	0	7	14964.14970	14964.15014	-0.00044
7	1	6	6	1	5	15221.67849	15221.67793	0.00056
7	3	5	6	3	4	15323.85829	15323.85847	-0.00018
7	5	3	6	5	2	15360.34509	15360.34492	0.00017
7	5	2	6	5	1	15363.57538	15363.57446	0.00092
7	4	4	6	4	3	15428.36110	15428.36343	-0.00233

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
7	4	3	6	4	2	15508.40309	15508.40353	-0.00044
7	3	4	6	3	3	16049.42328	16049.42275	0.00053
7	2	5	6	2	4	16397.08896	16397.08794	0.00102
8	2	7	7	2	6	16486.68701	16486.68703	-0.00002
9	1	9	8	1	8	16698.55761	16698.55649	0.00112
9	0	9	8	0	8	16713.67641	16713.67519	0.00122
8	1	7	7	1	6	16944.53806	16944.53808	-0.00002
8	3	6	7	3	5	17443.13678	17443.13605	0.00073
8	5	4	7	5	3	17611.08333	17611.08259	0.00074
8	5	3	7	5	2	17623.66393	17623.66256	0.00137
8	4	5	7	4	4	17679.26063	17679.26044	0.00019
8	4	4	7	4	3	17884.55874	17884.55795	0.00079

Table S30: *syn* 3-fluoroanisole (<sup>13</sup>C6)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
3	1	2	2	1	1	7041.47775	7041.47781	-0.00006
4	0	4	3	0	3	8055.29528	8055.29555	-0.00027
4	1	3	3	1	2	9287.82115	9287.82039	0.00076
4	1	4	3	1	3	7735.88261	7735.88378	-0.00117
4	2	2	3	2	1	9197.39487	9197.39610	-0.00123
4	2	3	3	2	2	8599.34479	8599.34393	0.00086
5	0	5	4	0	4	9801.67985	9801.67944	0.00041
5	1	4	4	1	3	11427.16144	11427.16210	-0.00066
5	1	5	4	1	4	9582.84243	9582.84221	0.00022
5	2	3	4	2	2	11673.05756	11673.05738	0.00018
5	2	4	4	2	3	10662.81308	10662.81420	-0.00112
6	0	6	5	0	5	11526.13871	11526.13883	-0.00012
6	1	6	5	1	5	11398.52448	11398.52494	-0.00046
6	2	5	5	2	4	12673.38603	12673.38648	-0.00045

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
4	3	2	3	3	1	8773.45170	8773.45033	0.00137
4	3	1	3	3	0	8819.11279	8819.11255	0.00024
5	4	2	4	4	1	10972.34338	10972.34378	-0.00040
5	4	1	4	4	0	10977.98972	10977.99083	-0.00111
5	3	3	4	3	2	10987.46167	10987.46207	-0.00040
5	3	2	4	3	1	11140.07438	11140.07481	-0.00043
6	3	4	5	3	3	13188.61579	13188.61501	0.00078
6	4	2	5	4	1	13235.69590	13235.69655	-0.00065
7	0	7	6	0	6	13258.89362	13258.89389	-0.00027
6	1	5	5	1	4	13421.77038	13421.77057	-0.00019
6	3	3	5	3	2	13561.16174	13561.16184	-0.00010
6	2	4	5	2	3	14103.51817	14103.51826	-0.00009
7	2	6	6	2	5	14627.91149	14627.91254	-0.00105
8	1	8	7	1	7	14971.38327	14971.38440	-0.00113
8	0	8	7	0	7	15004.20433	15004.20285	0.00148
7	1	6	6	1	5	15262.13488	15262.13493	-0.00005
7	5	3	6	5	2	15394.92798	15394.92727	0.00071
7	5	2	6	5	1	15398.11044	15398.11084	-0.00040
7	4	4	6	4	3	15462.96863	15462.96865	-0.00002
7	4	3	6	4	2	15542.21077	15542.21129	-0.00052
7	3	4	6	3	3	16081.89775	16081.89729	0.00046
7	2	5	6	2	4	16434.28449	16434.28431	0.00018
8	2	7	7	2	6	16528.81244	16528.81226	0.00018
9	1	9	8	1	8	16742.92938	16742.92872	0.00066
9	0	9	8	0	8	16758.29850	16758.29843	0.00007
8	1	7	7	1	6	16990.69373	16990.69334	0.00039
8	3	6	7	3	5	17484.47787	17484.47760	0.00027
8	5	4	7	5	3	17650.47307	17650.47209	0.00098
8	5	3	7	5	2	17662.87559	17662.87563	-0.00004

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
8	4	5	7	4	4	17718.96069	17718.96020	0.00049
8	4	4	7	4	3	17922.33720	17922.33701	0.00019

Table S31: *syn* 3-fluoroanisole (<sup>13</sup>C7)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
4	0	4	3	0	3	7967.20366	7967.20521	-0.00155
4	1	3	3	1	2	9137.79950	9137.79817	0.00133
4	1	4	3	1	3	7639.91318	7639.91328	-0.00010
4	2	3	3	2	2	8467.80723	8467.80660	0.00063
5	0	5	4	0	4	9702.09808	9702.09769	0.00039
5	1	5	4	1	4	9469.21501	9469.21626	-0.00125
5	2	3	4	2	2	11446.48971	11446.49059	-0.00088
5	2	4	4	2	3	10506.51584	10506.51585	-0.00001
6	0	6	5	0	5	11409.47380	11409.47441	-0.00061
6	1	6	5	1	5	11268.27658	11268.27668	-0.00010
6	2	5	5	2	4	12496.83096	12496.83262	-0.00166
4	3	2	3	3	1	8626.26130	8626.25929	0.00201
4	3	1	3	3	0	8665.14314	8665.13838	0.00476
4	2	2	3	2	1	9017.30417	9017.30451	-0.00034
5	4	2	4	4	1	10786.67281	10786.66841	0.00440
5	4	1	4	4	0	10791.17991	10791.17881	0.00110
5	3	3	4	3	2	10803.54334	10803.54416	-0.00082
5	3	2	4	3	1	10934.23184	10934.23314	-0.00130
5	1	4	4	1	3	11259.43024	11259.43133	-0.00109
6	3	4	5	3	3	12971.17626	12971.17765	-0.00139
6	4	3	5	4	2	12984.61275	12984.61272	0.00003
6	4	2	5	4	1	13004.47679	13004.47631	0.00048
7	1	7	6	1	6	13045.08434	13045.08500	-0.00066
7	0	7	6	0	6	13121.97914	13121.97931	-0.00017

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
6	1	5	5	1	4	13250.40552	13250.40651	-0.00099
6	3	3	5	3	2	13293.73432	13293.73534	-0.00102
6	2	4	5	2	3	13843.37628	13843.37738	-0.00110
7	2	6	6	2	5	14435.16090	14435.16147	-0.00057
8	1	8	7	1	7	14807.40457	14807.40485	-0.00028
8	0	8	7	0	7	14846.45855	14846.45899	-0.00044
7	1	6	6	1	5	15095.62089	15095.62054	0.00035
7	3	5	6	3	4	15113.50711	15113.50722	-0.00011
7	4	4	6	4	3	15196.12087	15196.12048	0.00039
7	4	3	6	4	2	15259.94159	15259.94175	-0.00016
7	3	4	6	3	3	15749.88230	15749.88380	-0.00150
7	2	5	6	2	4	16154.50339	16154.50395	-0.00056
8	2	7	7	2	6	16322.68482	16322.68504	-0.00022
9	1	9	8	1	8	16561.20914	16561.20822	0.00092
9	0	9	8	0	8	16580.13717	16580.13667	0.00050
8	1	7	7	1	6	16824.47824	16824.47712	0.00112
8	3	6	7	3	5	17215.86581	17215.86596	-0.00015
8	5	4	7	5	3	17344.45611	17344.45543	0.00068
8	5	3	7	5	2	17353.80509	17353.80386	0.00123
8	4	5	7	4	4	17413.53688	17413.53669	0.00019
8	4	4	7	4	3	17578.84361	17578.84363	-0.00002

Table S32: *syn* 3-fluoroanisole (<sup>18</sup>O)

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
4	0	4	3	0	3	7951.66333	7951.66450	-0.00117
4	1	4	3	1	3	7620.85804	7620.85880	-0.00076
5	0	5	4	0	4	9686.38776	9686.38945	-0.00169
5	1	5	4	1	4	9447.60465	9447.60552	-0.00087
4	2	2	3	2	1	8969.68718	8969.68729	-0.00011

J'	K <sub>a</sub> '	K <sub>c</sub> '	J''	K <sub>a</sub> ''	K <sub>c</sub> ''	v <sub>obs</sub> /MHz	v <sub>calc</sub> /MHz	v <sub>obs-calc</sub> /MHz
4	2	3	3	2	2	8437.10762	8437.10848	-0.00086
5	2	4	4	2	3	10470.94593	10470.94655	-0.00062
5	1	4	4	1	3	11220.65105	11220.65272	-0.00167
6	1	6	5	1	5	11244.47206	11244.47228	-0.00022
5	2	3	4	2	2	11386.36552	11386.36671	-0.00119
6	0	6	5	0	5	11391.42804	11391.42907	-0.00103
6	2	5	5	2	4	12457.96081	12457.96164	-0.00083
7	1	7	6	1	6	13019.07881	13019.07921	-0.00040
7	0	7	6	0	6	13100.26646	13100.26854	-0.00208
6	1	5	5	1	4	13214.30033	13214.30126	-0.00093
6	2	4	5	2	3	13775.40591	13775.40591	0.00000
7	2	6	6	2	5	14394.42246	14394.42169	0.00077
8	1	8	7	1	7	14778.99117	14778.98880	0.00237
7	1	6	6	1	5	15065.51512	15065.51455	0.00057
7	2	5	6	2	4	16083.67117	16083.66858	0.00259
8	2	7	7	2	6	16281.09531	16281.09444	0.00087
9	1	9	8	1	8	16530.12976	16530.12976	0.00000
9	0	9	8	0	8	16550.66163	16550.65973	0.00190
8	1	7	7	1	6	16799.11862	16799.11778	0.00084



### Appendix III: Kraitchman Coordinates

Table S33:  $r_s$  coordinates for *anti* 2-fluoroanisole

$^{13}\text{C1}$			
	a	b	
Planar	$0.47920 \pm 0.00001$	$0.08753 \pm 0.00003$	
+Costain err	$0.47920 \pm 0.00313$	$0.08753 \pm 0.01714$	
	a	b	c
Nonplanar	$0.47869 \pm 0.00002$	$0.08469 \pm 0.00009$	$0.02209 \pm 0.00035$
+Costain err	$0.47869 \pm 0.00313$	$0.08469 \pm 0.01771$	$0.02209 \pm 0.06792$
$^{13}\text{C2}$			
	a	b	
Planar	$0.44185 \pm 0.00001$	$0.89796 \pm 0.00000$	
+Costain err	$0.44185 \pm 0.00339$	$0.89796 \pm 0.00167$	
	a	b	c
Nonplanar	$0.44180 \pm 0.00002$	$0.89793 \pm 0.00001$	$0.00662 \pm 0.00117$
+Costain err	$0.44180 \pm 0.00340$	$0.89793 \pm 0.00167$	$0.00662 \pm 0.22645$
$^{13}\text{C3}$			
	a	b	
Planar	$1.81046 \pm 0.00000$	$0.65482 \pm 0.00000$	
+Costain err	$1.81046 \pm 0.00083$	$0.65482 \pm 0.00229$	
	a	b	c
Nonplanar	$1.81036 \pm 0.00000$	$0.65451 \pm 0.00001$	$0.02000 \pm 0.00037$
+Costain err	$1.81036 \pm 0.00083$	$0.65451 \pm 0.00229$	$0.02000 \pm 0.07500$
$^{13}\text{C4}$			
	a	b	
Planar	$2.26478 \pm 0.00000$	$0.66375 \pm 0.00000$	
+Costain err	$2.26478 \pm 0.00066$	$0.66375 \pm 0.00226$	

	a	b	c
Nonplanar	$2.26477 \pm 0.00000$	$0.66373 \pm 0.00001$	$0.00518 \pm 0.00165$
+Costain err	$2.26477 \pm 0.00066$	$0.66373 \pm 0.00226$	$0.00518 \pm 0.28931$
<hr/>			
<sup>13</sup> C5			
	a	b	
Planar	$1.34136 \pm 0.00001$	$1.70677 \pm 0.00000$	
+Costain err	$1.34136 \pm 0.00112$	$1.70677 \pm 0.00088$	
	a	b	c
Nonplanar	$1.34152 \pm 0.00001$	$1.70690 \pm 0.00000$	$0.02108*i \pm 0.00040$
+Costain err	$1.34152 \pm 0.00112$	$1.70690 \pm 0.00088$	$0.02108*i \pm 0.07115$
<hr/>			
<sup>13</sup> C6			
	a	b	
Planar	$0.08191*i \pm 0.00007$	$1.44480 \pm 0.00000$	
+Costain err	$0.08191*i \pm 0.01831$	$1.44480 \pm 0.00104$	
	a	b	c
Nonplanar	$0.08449*i \pm 0.00009$	$1.44465 \pm 0.00001$	$0.02103 \pm 0.00037$
+Costain err	$0.08449*i \pm 0.01775$	$1.44465 \pm 0.00104$	$0.02103 \pm 0.07134$
<hr/>			
<sup>13</sup> C7			
	a	b	
Planar	$2.77228 \pm 0.00000$	$0.77035 \pm 0.00000$	
+Costain err	$2.77228 \pm 0.00054$	$0.77035 \pm 0.00195$	
	a	b	c
Nonplanar	$2.77227 \pm 0.00000$	$0.77031 \pm 0.00001$	$0.00789 \pm 0.00106$
+Costain err	$2.77227 \pm 0.00054$	$0.77031 \pm 0.00195$	$0.00789 \pm 0.19022$
<hr/>			
<sup>18</sup> O			

	a	b	
Planar	1.79357 ± 0.00000	0.25795 ± 0.00001	
+Costain err	1.79357 ± 0.00084	0.25795 ± 0.00582	
	a	b	c
Nonplanar	1.79328 ± 0.00000	0.25575 ± 0.00002	0.03309 ± 0.00017
+Costain err	1.79328 ± 0.00084	0.25575 ± 0.00587	0.03309 ± 0.04533

Table S34:  $r_s$  coordinates for *anti* 3-fluoroanisole

$^{13}\text{C1}$			
	a	b	
Planar	0.83030 ± 0.00001	0.17497 ± 0.00003	
+Costain err	0.83030 ± 0.00181	0.17497 ± 0.00857	
	a	b	c
Nonplanar	0.83003 ± 0.00001	0.17368 ± 0.00006	0.02117 ± 0.00048
+Costain err	0.83003 ± 0.00181	0.17368 ± 0.00864	0.02117 ± 0.07084
$^{13}\text{C2}$			
	a	b	
Planar	0.29972 ± 0.00003	0.95684 ± 0.00001	
+Costain err	0.29972 ± 0.00500	0.95684 ± 0.00157	
	a	b	c
Nonplanar	0.29903 ± 0.00003	0.95663 ± 0.00001	0.02038 ± 0.00050
+Costain err	0.29903 ± 0.00502	0.95663 ± 0.00157	0.02038 ± 0.07359
$^{13}\text{C3}$			
	a	b	
Planar	1.53924 ± 0.00001	0.28908 ± 0.00002	
+Costain err	1.53924 ± 0.00097	0.28908 ± 0.00519	

	a	b	c
Nonplanar	1.53922 ± 0.00001	0.28895 ± 0.00003	0.00864 ± 0.00116
+Costain err	1.53922 ± 0.00097	0.28895 ± 0.00519	0.00864 ± 0.17356
<hr/>			
<sup>13</sup> C4			
	a	b	
Planar	1.65826 ± 0.00001	1.08516 ± 0.00001	
+Costain err	1.65826 ± 0.00090	1.08516 ± 0.00138	
	a	b	c
Nonplanar	1.65828 ± 0.00001	1.08518 ± 0.00001	0.00766*i ± 0.00134
+Costain err	1.65828 ± 0.00090	1.08518 ± 0.00138	0.00766*i ± 0.19595
<hr/>			
<sup>13</sup> C5			
	a	b	
Planar	0.47497 ± 0.00002	1.82682 ± 0.00001	
+Costain err	0.47497 ± 0.00316	1.82682 ± 0.00082	
	a	b	c
Nonplanar	0.47601 ± 0.00003	1.82710 ± 0.00001	0.03203*i ± 0.00044
+Costain err	0.47601 ± 0.00315	1.82710 ± 0.00082	0.03203*i ± 0.04684
<hr/>			
<sup>13</sup> C6			
	a	b	
Planar	0.77082 ± 0.00001	1.20469 ± 0.00000	
+Costain err	0.77082 ± 0.00195	1.20469 ± 0.00125	
	a	b	c
Nonplanar	0.77082 ± 0.00001	1.20469 ± 0.00001	0.00284 ± 0.00360
+Costain err	0.77082 ± 0.00195	1.20469 ± 0.00125	0.00284 ± 0.52788
<hr/>			
<sup>13</sup> C7			
	a	b	

Planar	$3.21727 \pm 0.00000$	$0.18593 \pm 0.00003$	
+Costain err	$3.21727 \pm 0.00047$	$0.18593 \pm 0.00807$	
	a	b	c
Nonplanar	$3.21713 \pm 0.00000$	$0.18340 \pm 0.00006$	$0.03045 \pm 0.00034$
+Costain err	$3.21713 \pm 0.00047$	$0.18340 \pm 0.00818$	$0.03045 \pm 0.04926$
<hr/>			
<sup>18</sup> O			
	a	b	
Planar	$1.99650 \pm 0.00000$	$0.90579 \pm 0.00001$	
+Costain err	$1.99650 \pm 0.00075$	$0.90579 \pm 0.00166$	
	a	b	c
Nonplanar	$1.99630 \pm 0.00000$	$0.90532 \pm 0.00001$	$0.02894 \pm 0.00025$
+Costain err	$1.99630 \pm 0.00075$	$0.90532 \pm 0.00166$	$0.02894 \pm 0.05183$
<hr/>			

Table S35: r<sub>s</sub> coordinates for *syn* 3-fluoroanisole

<sup>13</sup> C1			
	a	b	
Planar	$0.88482 \pm 0.00001$	$0.31856 \pm 0.00008$	
+Costain err	$0.88482 \pm 0.00170$	$0.31856 \pm 0.00471$	
	a	b	c
Nonplanar	$0.88466 \pm 0.00002$	$0.31811 \pm 0.00005$	$0.01699 \pm 0.00100$
+Costain err	$0.88466 \pm 0.00170$	$0.31811 \pm 0.00472$	$0.01699 \pm 0.08829$
<hr/>			
<sup>13</sup> C2			
	a	b	
Planar	$0.13902*i \pm 0.00006$	$0.77124 \pm 0.00003$	
+Costain err	$0.13902*i \pm 0.01079$	$0.77124 \pm 0.00195$	

	a	b	c
Nonplanar	$0.14197^*i \pm 0.00012$	$0.77069 \pm 0.00002$	$0.02888 \pm 0.00059$
+Costain err	$0.14197^*i \pm 0.01057$	$0.77069 \pm 0.00195$	$0.02888 \pm 0.05194$
<hr/>			
<sup>13</sup> C3			
	a	b	
Planar	$1.33223 \pm 0.00001$	$0.50823 \pm 0.00005$	
+Costain err	$1.33223 \pm 0.00113$	$0.50823 \pm 0.00295$	
	a	b	c
Nonplanar	$1.33221 \pm 0.00001$	$0.50818 \pm 0.00003$	$0.00706 \pm 0.00240$
+Costain err	$1.33221 \pm 0.00113$	$0.50818 \pm 0.00295$	$0.00706 \pm 0.21237$
<hr/>			
<sup>13</sup> C4			
	a	b	
Planar	$1.87906 \pm 0.00000$	$0.75294 \pm 0.00003$	
+Costain err	$1.87906 \pm 0.00080$	$0.75294 \pm 0.00199$	
	a	b	c
Nonplanar	$1.87896 \pm 0.00001$	$0.75268 \pm 0.00002$	$0.01955 \pm 0.00088$
+Costain err	$1.87896 \pm 0.00080$	$0.75268 \pm 0.00199$	$0.01955 \pm 0.07671$
<hr/>			
<sup>13</sup> C5			
	a	b	
Planar	$0.98466 \pm 0.00001$	$1.83455 \pm 0.00001$	
+Costain err	$0.98466 \pm 0.00152$	$1.83455 \pm 0.00082$	
	a	b	c
Nonplanar	$0.98495 \pm 0.00002$	$1.83471 \pm 0.00001$	$0.02426^*i \pm 0.00070$
+Costain err	$0.98495 \pm 0.00152$	$1.83471 \pm 0.00082$	$0.02426^*i \pm 0.06182$
<hr/>			
<sup>13</sup> C6			
	a	b	
Planar	$0.38229 \pm 0.00002$	$1.62958 \pm 0.00002$	

+Costain err	$0.38229 \pm 0.00392$	$1.62958 \pm 0.00092$	
	a	b	c
Nonplanar	$0.38282 \pm 0.00004$	$1.62971 \pm 0.00001$	$0.02046*i \pm 0.00084$
+Costain err	$0.38282 \pm 0.00392$	$1.62971 \pm 0.00092$	$0.02046*i \pm 0.07333$
<hr/>			
<sup>13</sup> C7			
	a	b	
Planar	$2.80962 \pm 0.00000$	$1.08243 \pm 0.00003$	
+Costain err	$2.80962 \pm 0.00053$	$1.08243 \pm 0.00139$	
	a	b	c
Nonplanar	$2.80960 \pm 0.00001$	$1.08237 \pm 0.00002$	$0.01095 \pm 0.00164$
+Costain err	$2.80960 \pm 0.00053$	$1.08237 \pm 0.00139$	$0.01095 \pm 0.13696$
<hr/>			
<sup>18</sup> O			
	a	b	
Planar	$2.25073 \pm 0.00000$	$0.22232 \pm 0.00008$	
+Costain err	$2.25073 \pm 0.00067$	$0.22232 \pm 0.00675$	
	a	b	c
Nonplanar	$2.25054 \pm 0.00000$	$0.22019 \pm 0.00005$	$0.03038 \pm 0.00036$
+Costain err	$2.25054 \pm 0.00067$	$0.22019 \pm 0.00681$	$0.03038 \pm 0.04938$
<hr/>			

## Appendix IV: Ground State Effective Structures (r<sub>0</sub>)

Table S36. r<sub>0</sub> structural parameters for *anti* 2-fluoroanisole

	r <sub>0</sub> #1	r <sub>0</sub> #2
C1-C2	1.407(8)	1.393(10)
C2-C3	1.377(4)	1.386(3)
C3-C4	1.405(7)	1.405(7)
C4-C5	1.390(4)	1.388(4)
C5-C6	1.414(9)	1.411(9)
C6-C1	1.390(8)	1.400(13)
C1-O	1.364(7)	1.358(8)
O-C7	1.434(4)	1.427(6)
<(C1-C2-C3)	122.3(4)	122.4(5)
<(C2-C3-C4)	119.0(3)	119.0(3)
<(C3-C4-C5)	119.6(2)	119.6(2)
<(C4-C5-C6)	120.9(2)	120.9(2)
<(C5-C6-C1)	119.5(5)	119.6(5)
<(C6-C1-C2)	118.6(6)	118.5(6)
<(C2-C1-O)	115.3(6)	116.0(9)
<(C1-O-C7)	115.9(4)	116.8(7)

Table S36. r<sub>0</sub> structural parameters for *anti* 3-fluoroanisole

	r <sub>0</sub> #1	r <sub>0</sub> #2
C1-C2	1.399(12)	1.401(13)
C2-C3	1.389(6)	1.389(8)
C3-C4	1.395(4)	1.394(4)
C4-C5	1.388(7)	1.387(6)
C5-C6	1.412(8)	1.413(7)
C6-C1	1.387(19)	1.386(19)
C1-O	1.370(10)	1.370(11)
O-C7	1.419(5)	1.419(5)



	r <sub>0</sub> #1	r <sub>0</sub> #2
<(C1-C2-C3)	117.7(7)	117.7(7)
<(C2-C3-C4)	123.2(3)	123.2(3)
<(C3-C4-C5)	117.4(3)	117.4(2)
<(C4-C5-C6)	121.7(2)	121.7(2)
<(C5-C6-C1)	118.5(3)	118.5(3)
<(C6-C1-C2)	121.6(7)	121.5(7)
<(C2-C1-O)	113.8(13)	113.8(13)
<(C1-O-C7)	117.2(7)	117.17(8)

Table S37. r<sub>0</sub> structural parameters for *syn* 3-fluoroanisole

	r <sub>0</sub> #1	r <sub>0</sub> #2
C1-C2	1.392(10)	1.401(11)
C2-C3	1.400(10)	1.392(10)
C3-C4	1.387(5)	1.382(4)
C4-C5	1.399(4)	1.399(4)
C5-C6	1.399(8)	1.407(8)
C6-C1	1.396(9)	1.394(9)
C1-O	1.365(4)	1.363(4)
O-C7	1.428(6)	1.426(6)
<(C1-C2-C3)	117.0(5)	117.3(5)
<(C2-C3-C4)	123.8(3)	124.1(3)
<(C3-C4-C5)	117.2(2)	117.3(2)
<(C4-C5-C6)	121.2(2)	121.2(2)
<(C5-C6-C1)	119.3(4)	119.1(4)
<(C6-C1-C2)	121.5(5)	121.1(6)
<(C2-C1-O)	123.5(7)	123.8(8)
<(C1-O-C7)	117.3(5)	117.4(5)