

## Supplemental Material

Gas phase measurements of mono-fluoro-benzoic acids and the dimer of 3-fluoro-benzoic acid.

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Table S1. The measured transitions for 2-Fluorobenzoic acid conformer 1 from 3.9 GHz to 10.7 GHz. Frequencies and Experimental – Calculated (Exp-Calc) frequencies in MHz.

J'	K' <sub>a</sub>	K' <sub>c</sub>	J''	K'' <sub>a</sub>	K'' <sub>c</sub>	obs	o-c	est. unc.
4	1	4	3	0	3	7210.572	0.0051	0.005
5	1	5	4	0	4	8361.202	0.0006	0.005
6	0	6	5	1	5	8385.847	0.0029	0.005
5	0	5	4	1	4	6721.795	0.0068	0.005
9	3	6	9	2	7	7286.028	-0.0128	0.005
7	1	6	6	2	5	8402.189	0.0032	0.005
9	2	7	8	3	6	8431.505	-0.0231	0.005
7	1	6	7	0	7	6671.145	0.0159	0.005
5	2	4	5	1	5	7484.536	0.0128	0.005
8	3	5	8	2	6	7639.777	-0.0099	0.005
9	2	7	9	1	8	6281.034	-0.0141	0.005
6	1	5	5	2	4	6231.616	0.0086	0.005
4	0	4	3	0	3	6250.942	0.0102	0.005
4	1	3	3	1	2	6890.148	0.0041	0.005
10	3	7	10	2	8	7104.434	-0.005	0.005
5	1	5	4	1	4	7401.563	-0.0032	0.005

Table S2. The measured transitions for 2-Fluorobenzoic acid conformer 2 from 3.9 GHz to 10.7 GHz. Frequencies and Experimental – Calculated (Exp-Calc) frequencies in MHz.

J'	K' <sub>a</sub>	K' <sub>c</sub>	J''	K'' <sub>a</sub>	K'' <sub>c</sub>	obs	o-c	est. unc.
4	1	4	3	1	3	7013.59	0.0046	0.05
4	0	4	3	0	3	7231.601	0.0038	0.005
3	1	2	2	1	1	6571.283	0.0033	0.005
5	1	5	4	1	4	8658.288	-0.0002	0.005
5	0	5	4	0	4	8776.137	0.0038	0.005
5	1	4	4	1	3	10464.7	-0.0051	0.005
4	0	4	3	1	3	6803.93	0.0015	0.005
4	1	4	3	0	3	7441.253	-0.0006	0.005
5	0	5	4	1	4	8566.474	-0.0024	0.005

5	1	5	4	0	4	8867.947	0.0021	0.005
6	1	6	5	1	5	10273.75	-0.0055	0.005
3	2	2	2	2	1	6014.657	0.0065	0.005
4	2	2	3	2	1	8724.595	-0.0017	0.005

Table S3. The measured transitions for 2-Fluorobenzoic acid conformer 3 from 3.9 GHz to 10.7 GHz. Frequencies and Experimental – Calculated (Exp-Calc) frequencies in MHz.

J'	K' <sub>a</sub>	K' <sub>c</sub>	J''	K'' <sub>a</sub>	K'' <sub>c</sub>	obs	o-c	est. unc.
4	1	4	3	1	3	7011.251	0.0025	0.005
4	0	4	3	0	3	7233.289	0.0005	0.005
3	1	2	2	1	1	6564.786	0.0049	0.005
5	1	5	4	1	4	8656.414	0.0026	0.005
5	0	5	4	0	4	8777.774	0.0004	0.005
5	1	4	4	1	3	10463.71	-0.0049	0.005
4	0	4	3	1	3	6793.689	0.0002	0.005
4	1	4	3	0	3	7450.852	0.0038	0.005
5	0	5	4	1	4	8560.213	-0.0013	0.005
5	1	5	4	0	4	8873.971	-0.0004	0.005
6	1	6	5	1	5	10272.19	-0.0041	0.005
3	2	2	2	2	1	6008.899	0.0004	0.005
4	2	2	3	2	1	8709.091	-0.0003	0.005
5	2	4	5	0	5	7317.028	0.0094	0.005
7	4	3	7	3	4	7318.847	-0.0152	0.005

Table S4. The measured transitions for 3-Fluorobenzoic acid conformer 1 from 3.9 GHz to 10.7 GHz. Frequencies and Experimental – Calculated (Exp-Calc) frequencies in MHz.

J'	K' <sub>a</sub>	K' <sub>c</sub>	J''	K'' <sub>a</sub>	K'' <sub>c</sub>	obs	o-c	est. unc.
5	0	5	4	0	4	7711.977	-0.0012	0.005
5	1	5	4	1	4	7438.504	0.0011	0.005
4	1	3	3	1	2	6952.571	0.0032	0.005
4	0	4	3	0	3	6282.712	0.0003	0.005
6	0	6	5	0	5	9095.441	0.0014	0.005
6	1	6	5	1	5	8879.271	-0.0015	0.005
5	1	4	4	1	3	8633.505	-0.0028	0.005

Table S5. The measured transitions for 3-Fluorobenzoic acid conformer 2 from 3.9 GHz to 10.7 GHz. Frequencies and Experimental – Calculated (Exp-Calc) frequencies in MHz.

J'	K' <sub>a</sub>	K' <sub>c</sub>	J''	K'' <sub>a</sub>	K'' <sub>c</sub>	obs	o-c	est. unc.
4	1	4	3	0	3	7210.572	0.0051	0.005
5	1	5	4	0	4	8361.202	0.0006	0.005
6	0	6	5	1	5	8385.847	0.0029	0.005
5	0	5	4	1	4	6721.795	0.0068	0.005
9	3	6	9	2	7	7286.028	-0.0128	0.005
7	1	6	6	2	5	8402.189	0.0032	0.005
9	2	7	8	3	6	8431.505	-0.0231	0.005
7	1	6	7	0	7	6671.145	0.0159	0.005
5	2	4	5	1	5	7484.536	0.0128	0.005
8	3	5	8	2	6	7639.777	-0.0099	0.005
9	2	7	9	1	8	6281.034	-0.0141	0.005
6	1	5	5	2	4	6231.616	0.0086	0.005
4	0	4	3	0	3	6250.942	0.0102	0.005
4	1	3	3	1	2	6890.148	0.0041	0.005
10	3	7	10	2	8	7104.434	-0.005	0.005
5	1	5	4	1	4	7401.563	-0.0032	0.005

Table S6. The measured transitions for 3FBenzoic Acid-Formic Acid dimmer from 3.9 GHz to 10.7 GHz. Frequencies and Experimental – Calculated (Exp-Calc) frequencies in MHz.

n	J'	Ka	Kc	v'	J''	Ka	Kc	v''	Exp. FREQUENCY	Exp-Calc
1	4	2	3	0	3	1	2	0	3908.6720	0.0077
2	5	2	4	0	4	1	3	0	4077.9409	0.0091
3	5	2	3	0	4	1	4	0	4151.2974	-0.0004
4	6	2	5	0	5	1	4	0	4243.6079	-0.0033
5	7	2	6	0	6	1	5	0	4405.6780	-0.0504
6	7	2	6	1	6	1	5	1	4406.0080	0.0559
7	4	3	1	0	4	2	2	0	5325.5370	0.0276
8	5	3	3	1	5	2	4	1	5326.2460	0.0024
9	5	3	3	0	5	2	4	0	5326.3100	0.0483
10	6	3	4	1	6	2	5	1	5326.5930	-0.0045
11	6	3	4	0	6	2	5	0	5326.6680	0.0520
12	3	3	0	0	2	2	1	0	5876.9560	-0.0162
13	4	3	2	0	3	2	1	0	6060.5098	-0.0099
14	4	3	2	1	3	2	1	1	6060.5620	0.0047
15	4	3	1	0	3	2	2	0	6060.7021	-0.0019

16	4	3	1	1	3	2	2	1	6060.7544	0.0144
17	5	3	3	0	4	2	2	0	6243.9473	-0.0100
18	5	3	3	1	4	2	2	1	6244.0430	0.0107
19	5	3	2	0	4	2	3	0	6244.5000	-0.0126
20	5	3	2	1	4	2	3	1	6244.5967	0.0163
21	6	3	4	1	5	2	3	1	6427.2627	-0.0079
22	6	3	3	0	5	2	4	0	6428.4399	-0.0111
23	6	3	3	1	5	2	4	1	6428.5537	0.0041
24	7	3	5	0	6	2	4	0	6609.9805	0.0069
25	7	3	5	1	6	2	4	1	6610.1279	-0.0140
26	7	3	4	0	6	2	5	0	6612.5908	0.0055
27	7	3	4	1	6	2	5	1	6612.7100	0.0088
28	8	3	5	0	7	2	6	0	6796.9897	-0.0020
29	8	3	5	1	7	2	6	1	6797.1191	0.0189
30	8	3	6	0	7	2	5	0	6792.2876	0.0096
31	8	3	6	1	7	2	5	1	6792.4731	-0.0159
32	9	3	7	1	8	2	6	1	6974.1226	-0.0067
33	5	4	1	1	5	3	2	1	7456.1600	-0.0097
34	4	4	0	0	3	3	1	0	8190.9900	0.0047
35	4	4	1	1	3	3	0	1	8191.0040	-0.0085
36	5	4	2	0	4	3	1	0	8374.6328	-0.0086
37	5	4	2	1	4	3	1	1	8374.6999	-0.0038
38	6	4	3	0	5	3	2	0	8558.2860	0.0030
39	6	4	3	1	5	3	2	1	8558.3850	-0.0013
40	7	4	4	0	6	3	3	0	8741.9200	0.0147
41	7	4	4	1	6	3	3	1	8742.0520	0.0064
42	5	5	0	0	4	4	1	0	10504.9627	-0.0396
43	5	5	0	1	4	4	1	1	10505.0050	-0.0478
44	6	5	1	0	5	4	2	0	10688.6480	-0.0025
45	6	5	1	1	5	4	2	1	10688.7120	-0.0345
46	7	5	2	0	6	4	3	0	10872.3060	0.0135
47	7	5	2	1	6	4	3	1	10872.4160	-0.0175
48	8	5	4	0	7	4	3	0	11055.9450	0.0140
49	8	5	4	1	7	4	3	1	11056.0850	-0.0178
50	9	5	5	0	8	4	4	0	11239.5760	0.0085
51	9	5	5	1	8	4	4	1	11239.7590	0.0161
52	6	6	0	0	5	5	1	0	12819.0040	0.0012

Table S7. The measured transitions for 4-Fluorobenzoic acid from 3.9 GHz to 10.7 GHz.

Frequencies and Experimental – Calculated (Exp-Calc) frequencies in MHz.

J'	K' <sub>a</sub>	K' <sub>c</sub>	J''	K'' <sub>a</sub>	K'' <sub>c</sub>	obs	o-c	est. unc.
3	1	3	2	0	2	7022.621	0.0017	0.005
4	1	4	3	0	3	8193.05	-0.001	0.005
5	1	5	4	0	4	9313.598	-0.0012	0.005
6	1	6	5	0	5	10395.29	0.0006	0.005
7	1	7	6	0	6	11451.38	0.0003	0.005
6	0	6	5	1	5	6104.355	0.0019	0.005
7	0	7	6	1	6	7731.522	-0.0017	0.005