Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for

Rotational spectroscopy of the atmospheric photo-oxidation product o-toluic acid and its monohydrate

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Table S1 Measured transition frequencies of *o*-toluic acid monomer

J'	K_a'	K_c'	*J"*	K_a"	K_c"	Frequency/MHz	Residual[a]/MHz
3	1	2	2	1	1	6551.3821	-0.0003
4	1	4	3	1	3	6976.9249	-0.0002
4	0	4	3	0	3	7180.5499	-0.0005
4	2	3	3	2	2	7909.3256	-0.0003
4	3	2	3	3	1	8166.7224	0.0007
4	3	1	3	3	0	8268.7504	-0.0025
8	2	6	8	1	7	8321.3193	-0.0004
6	2	5	6	1	6	8370.8383	-0.0010
5	4	2	5	3	3	8386.4772	-0.0006
6	4	3	6	3	4	8494.9656	-0.0001
7	3	5	7	2	6	8499.7610	0.0017
5	0	5	4	1	4	8531.6256	-0.0002
4	1	3	3	1	2	8565.3368	0.0006
5	1	5	4	1	4	8609.7272	-0.0003
5	0	5	4	0	4	8715.8030	0.0002
4	2	2	3	2	1	8720.7769	0.0011
5	1	5	4	0	4	8793.9037	-0.0009
8	4	5	8	3	6	9244.3895	0.0003
8	3	6	8	2	7	9653.9507	-0.0004
5	2	4	4	2	3	9755.1041	0.0002
6	1	6	5	1	5	10214.0190	0.0004
5	3	3	4	3	2	10215.9616	0.0007
6	0	6	5	0	5	10261.3046	0.0001
5	1	4	4	1	3	10401.2061	0.0010
5	3	2	4	3	1	10537.2328	0.0003
5	2	3	4	2	2	11013.4340	0.0009
6	2	5	5	2	4	11527.6311	0.0007
7	0	7	6	1	6	11790.9173	-0.0005
7	1	7	6	1	6	11802.5072	-0.0002
7	0	7	6	0	6	11821.7334	-0.0004
7	1	7	6	0	6	11833.3232	-0.0002
6	1	5	5	1	4	12041.7618	0.0001
6	3	4	5	3	3	12225.1508	0.0010
6	4	3	5	4	2	12333.6379	0.0002
6	4	2	5	4	1	12414.0476	-0.0015
6	3	3	5	3	2	12930.1272	-0.0006
8	0	8	7	1	7	13379.2282	0.0000
8	1	8	7	1	7	13383.4407	-0.0004
8	0	8	7	0	7	13390.8185	0.0007
8	1	8	7	0	7	13395.0308	0.0001

[a] (Measured transition frequency) – (Fit transition frequency).

Table S2 Measured transition frequencies of *o*-toluic acid monohydrate

J'	K_a'	K_c'	*J"*	K_a"	K_c"	Frequency/MHz	Residual[a]/MHz
5	1	5	4	1	4	5308.6728	0.0003
5	0	5	4	0	4	5525.8203	-0.0007
5	2	4	4	2	3	5682.3695	-0.0006
5	2	3	4	2	2	5859.7853	-0.0004
5	1	4	4	1	3	6015.0663	-0.0006
5	1	5	4	0	4	6329.6376	0.0005
6	1	6	5	1	5	6349.9946	-0.0009
6	0	6	5	0	5	6551.0898	-0.0007
6	2	5	5	2	4	6801.652	-0.0001
6	2	4	5	2	3	7094.0887	0.0006
6	1	5	5	1	4	7185.9722	0.0014
7	1	7	6	1	6	7383.0492	-0.0003
7	0	7	6	0	6	7553.2356	0.0020
7	2	6	6	2	5	7911.7895	0.0009
7	3	5	6	3	4	8040.5871	0.0000
7	3	4	6	3	3	8087.9626	0.0000
7	1	6	6	1	5	8335.9875	0.0009
7	2	5	6	2	4	8341.6283	-0.0009
8	1	8	7	1	7	8408.3638	-0.0006
8	0	8	7	0	7	8541.8123	0.0006
8	1	8	7	0	7	8840.9011	-0.0004
4	2	3	3	1	2	8992.777	0.0000
8	2	7	7	2	6	9011.5757	-0.0014
8	3	6	7	3	5	9194.9882	0.0007
8	3	5	7	3	4	9286.9634	0.0002
9	1	9	8	1	8	9426.8718	0.0005
8	1	7	7	1	6	9459.5335	-0.0003
9	0	9	8	0	8	9525.2848	-0.0001
8	2	6	7	2	5	9590.7447	-0.0004
9	1	9	8	0	8	9725.9603	-0.0009
9	2	8	8	2	7	10100.0821	0.0004
10	1	10	9	1	9	10439.7173	0.0000
10	0	10	9	0	9	10508.9374	0.0009
9	1	8	8	1	7	10551.4965	-0.0007
9	2	7	8	2	6	10830.4742	0.0001
11	1	11	10	1	10	11448.0896	-0.0004

[a] (Measured transition frequency) – (Fit transition frequency).

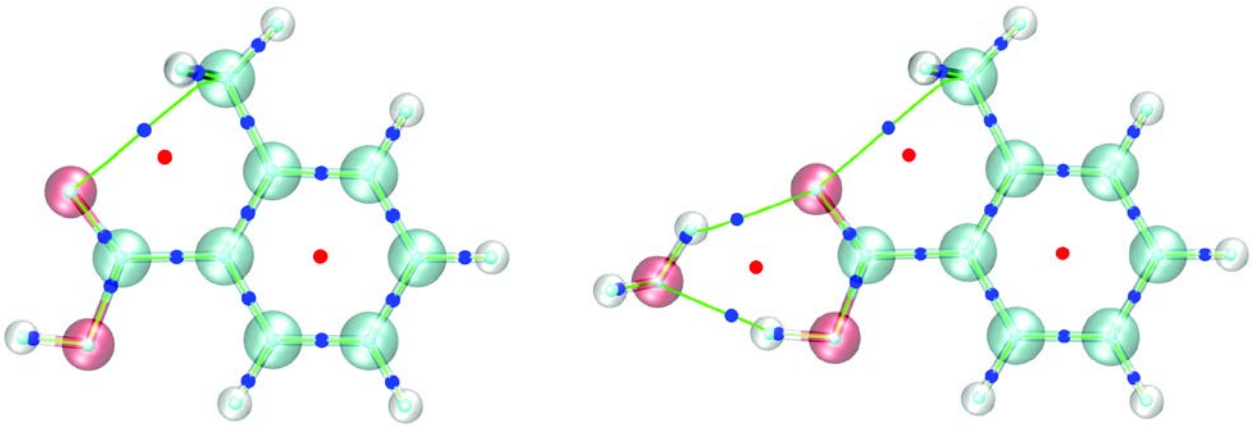

Fig. S1 Molecular graphs of *o*-toluic acid monomer and monohydrate, calculated at the MP2/6-311++G(2df,2pd) level of theory. Bond critical points are shown in blue, and ring critical points are shown in red.