Modifying conformational distribution of chiral tetrahydro-2-furoic acid through its interaction with water: a rotational spectroscopic and theoretical investigation

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Supplementary Information

Table of Contents

Table S1. Measured transition frequencies of **II**-9.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν_{EXP} / MHz	$\Delta\nu$[a] / MHz
1	0	1	0	0	0	2096.6412	0.0029
3	2	1	3	1	2	2405.2128	0.0018
4	2	2	4	1	3	2479.8702	0.0077
2	2	0	2	1	1	2550.9933	0.0063
1	1	1	0	0	0	2922.2378	-0.0058
4	1	3	4	1	4	3070.8364	0.0058
4	1	3	4	0	4	3243.2332	0.0040
2	0	2	1	1	1	3293.4864	0.0013
2	2	1	2	1	2	3421.0004	-0.0023
6	3	3	6	2	4	3660.0940	0.0052
6	2	4	6	1	5	3665.2280	-0.0020
7	3	4	7	2	5	3708.4830	0.0014
2	1	2	1	1	1	3878.5427	0.0036
5	3	2	5	2	3	3908.9209	0.0021
3	2	2	3	1	3	3935.0608	-0.0062
2	0	2	1	0	1	4119.0923	0.0018
3	2	2	3	0	3	4279.1002	-0.0038
4	3	1	4	2	2	4288.1001	0.0022
2	1	1	1	1	0	4507.9960	-0.0042
3	3	0	3	2	1	4620.8580	0.0010
4	2	3	4	1	4	4626.5661	0.0049
2	1	2	1	0	1	4704.1443	-0.0001
4	2	3	4	0	4	4798.9540	-0.0058
3	3	1	3	2	2	4956.7762	-0.0024
4	3	2	4	2	3	5135.8011	0.0003
3	0	3	2	1	2	5431.7885	0.0005
5	3	3	5	2	4	5459.4390	-0.0051
5	2	4	5	1	5	5480.2012	0.0025
7	4	3	7	3	4	5646.3659	-0.0035
3	1	3	2	1	2	5775.8281	0.0031
3	0	3	2	0	2	6016.8418	-0.0002
6	4	2	6	3	3	6149.3160	0.0030
3	2	2	2	2	1	6289.8866	-0.0027
3	1	3	2	0	2	6360.8789	-0.0001
3	2	1	2	2	0	6562.9311	0.0002
3	1	2	2	1	1	6708.7057	-0.0012
6	1	5	6	0	6	5883.7272	-0.0004
6	3	4	6	2	5	5954.8264	-0.0027

[a] $\Delta\nu = \nu_{exp} - \nu_{cacl}$.

Table S2. Measured transition frequencies of **I**-10.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν_{EXP} / MHz	$\Delta\nu$[a] / MHz
1	0	1	0	0	0	2096.6412	0.0029
3	2	1	3	1	2	2405.2128	0.0018
4	2	2	4	1	3	2479.8702	0.0077
2	2	0	2	1	1	2550.9933	0.0063
1	1	1	0	0	0	2922.2378	-0.0058
4	1	3	4	1	4	3070.8364	0.0058
4	1	3	4	0	4	3243.2332	0.0040
2	0	2	1	1	1	3293.4864	0.0013
2	2	1	2	1	2	3421.0004	-0.0023
6	3	3	6	2	4	3660.094	0.0052
6	2	4	6	1	5	3665.228	-0.0020
7	3	4	7	2	5	3708.483	0.0014
2	1	2	1	1	1	3878.5427	0.0036
5	3	2	5	2	3	3908.9209	0.0021
3	2	2	3	1	3	3935.0608	-0.0062
2	0	2	1	0	1	4119.0923	0.0018
3	2	2	3	0	3	4279.1002	-0.0038
4	3	1	4	2	2	4288.1001	0.0022
2	1	1	1	1	0	4507.996	-0.0042
3	3	0	3	2	1	4620.858	0.0010
4	2	3	4	1	4	4626.5661	0.0049
2	1	2	1	0	1	4704.1443	-0.0001
4	2	3	4	0	4	4798.954	-0.0058
3	3	1	3	2	2	4956.7762	-0.0024
4	3	2	4	2	3	5135.8011	0.0003
3	0	3	2	1	2	5431.7885	0.0005
5	3	3	5	2	4	5459.439	-0.0051
5	2	4	5	1	5	5480.2012	0.0025
7	4	3	7	3	4	5646.3659	-0.0035
3	1	3	2	1	2	5775.8281	0.0031
3	0	3	2	0	2	6016.8418	-0.0002
6	4	2	6	3	3	6149.316	0.0030
3	2	2	2	2	1	6289.8866	-0.0027
3	1	3	2	0	2	6360.8789	-0.0001
3	2	1	2	2	0	6562.9311	0.0002
3	1	2	2	1	1	6708.7057	-0.0012
6	1	5	6	0	6	5883.7272	-0.0004
6	3	4	6	2	5	5954.8264	-0.0027

[a] $\Delta\nu = \nu_{exp} - \nu_{cacl}$.

Point S1. We estimate the anticipated signal-to-noise ratio of the strongest transition of **Type 1** monohydrate, **III-**1 (the global minimum) using the following steps.

1. The ***strongest*** observed transition of **I-**10 in the experimental region is 202-101 at 4119.0923 MHz with a signal-to-noise ratio of 181 and that of **II-**9 is 202-101 at 3998.9497 MHz with a signal-to-noise ratio of 167. The corresponding line intensities of **I-**10 and **II-**9 predicted, using Pgopher with the experimentally determined spectroscopic constants, the calculated permanent electric dipole moment components, and an estimated rotational temperature of 1 K, are 0.0082 and 0.0085 (arbitrary unit), respectively.

2. The ***strongest*** transition on the non-observed **Type 1** structure, the global minimum **III-**1 structure, is 110-000 at 4111.99 MHz whose Pgopher predicted line intensity is 0.000135 (arbitrary unit).

3. The experimental abundance ratio of the *trans*- versus *cis*-THFA monomer is about 10 : 1~2. We use a ratio of 10 : 1.5 below for simplicity.

It is known from the "argon-test" experiments reported in Ref. 32 that the conversion from **III** to **I** and **II** rarely happens in a jet expansion. The barrier of conversion from **Type 1** (or more specifically **III-**1) to **Type 2** (**II-**9 and **I-**10) remains high and the conversion from **Type 1** to **Type 2** structures can be considered as forbidden in a jet expansion, as discussed in detail in the main text. The anticipated (upper limit) signal-to-noise ratio of the strongest transition of **III-**1 can be estimated based on the above information:

$$181 \times (1.5/10) \times (0.000135/0.0082) \approx 0.4 \text{ based on } \mathbf{I}\text{-}10$$
$$167 \times (1.5/10) \times (0.000135/0.0085) \approx 0.4 \text{ based on } \mathbf{II}\text{-}9$$

The above numbers justify why we were not able to detect **III-**1, the global minimum.