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

Conformational equilibrium and internal dynamics in the *iso*-propanol-water dimer

Electronic Supplementary Information

Content:

- 2 Tables of experimental transition frequencies
- 1 Table of MP2/6-311++G(d,p) principal axes coordinates (Å) with the *ab initio* geometry of the observed conformer, and related sketch.

Table S1. Experimental transition frequencies (ν, MHz) of the parent and 4 isotopologues of the *GAI* conformer of isopropanol-water.

$J'(K_a',K_c')\leftarrow J''(K_a'',K_c'')$	v=0	v=1
2(0,2)-1(0,1)	9672.9654	9669.6825
2(1,2)-1(1,1)	9545.6430	9543.8442
2(1,1)-1(1,0)	9808.6429	9807.2838
3(0,3)-2(0,2)	14496.9525	14492.0836
3(1,3)-2(1,2)	14312.3465	14315.0518
3(1,2)-2(1,1)	14709.4494	14707.3279
1(1,0)-0(0,0)	7583.8126	7584.4518
2(1,1)-1(0,1)	12553.4666	12554.3665
2(2,1)-1(1,1)	17779.5465	17784.4985
2(2,0)-1(1,0)	17652.8346	17657.6237
2(2,0)-2(1,2)	8238.6908	8245.5163
2(2,1)-2(1,1)	7839.4106	
3(0,3)-2(1,1)	11616.4511	11607.3970
3(1,2)-2(0,2)	17589.9498	17592.0134
3(2,1)-3(1,3)	8454.6958	8471.4178
3(2,2)-3(1,2)	7641.9066	
4(0,4)-3(1,2)	16213.1693	16200.3656
5(2,3)-5(1,5)	9193.3173	

Table S2. Experimental transition frequencies (ν, MHz) of the parent and 4 isotopologues of the *GAO* conformer of isopropanol-water.

$J'(K_a',K_c')\leftarrow J''(K_a'',K_c'')$	IP--H_2O	P--$H_2{}^{18}O$	IP--DOH	IP--HOD	IP--D_2O
1(1,1)-0(0,0)	9663.4408	9566.4109	9626.7537	9538.0977	
1(1,0)-0(0,0)	9967.7738	9837.8428			
2(0,2)-1(0,1)	7577.3284	7160.8101	7480.8164	7275.3624	7185.5180
2(1,2)-1(0,1)	13153.6133	12879.9932	13075.1366	12902.7078	
2(1,2)-1(1,1)	7284.6824	6898.5838	7194.3707	7007.1821	
2(1,1)-1(0,1)	13153.6133				
2(1,1)-1(1,0)	7893.3304	7441.4085	7789.5391	7563.1586	
3(0,3)-2(0,2)	11336.8526	10718.2997	11193.3981	10888.6704	10754.9739
3(1,3)-2(1,2)	10919.5307	10341.9229	10784.4189	10504.4255	10377.7389
3(1,2)-2(1,1)	11832.1992	11155.9409	11676.8869	11338.1684	11194.5952
3(2,2)-2(2,1)	11383.7359				
3(2,1)-2(2,0)	11429.7388				
4(0,4)-3(0,3)	15062.0568	14248.6851	14873.1901	14296.8917	
4(1,4)-3(1,3)	13778.3909		13994.3683	13826.0189	
4(1,3)-3(1,2)	15761.3331	14862.8111	15554.9606	15104.9914	14914.1840
4(2,3)-3(2,2)	15168.5536				
4(2,2)-3(2,1)	15282.8167				
5(0,5)-4(0,4)	17744.1676	18511.0642	18020.7238	17803.3600	
5(1,5)-4(1,4)	17206.1246	17937.7212	17475.0502	17265.4669	
5(1,4)-4(1,3)	18559.0192				

Table S3. MP2/6-311++G(d, p) geometry of the observed conformer of the *GAI* conformer of Isopropanol-water

bond lengths/Å		angles/°		dihedral angel/°	
C2C1	1.5225				
O3C2	1.4428	O3C2C1	106.4		
C4C2	1.5179	C4C2O3	110.5	C4C2O3C1	-122.4
O5O3	2.8537	O5O3C2	106.5	O5O3C2C1	60.5
H6O3	0.9630	H6O3C2	107.4	H6O3C2C1	179.6
H7C2	1.0984	H7C2O3	108.3	H7C2O3O5	177.9
H8C1	1.0937	H8C1C2	110.0	H8C1C2C4	-62.4
H9C1	1.0930	H9C1C2	110.3	H9C1C2C4	177.7
H10C1	1.0937	H10C1C2	110.0	H10C1C2C4	57.4
H11C4	1.0944	H11C4C2	110.3	H11C4C2C1	61.1
H12C4	1.0956	H12C4C2	111.0	H12C4C2C1	-179.3
H13C4	1.0939	H13C4C2	109.9	H13C4C2C1	-59.1
H14O5	0.9688	H14O5O3	8.3	H14O5O3C2	-146.3
H15O5	0.9590	H15O5O3	112.2	H15O5O3C2	-141.0

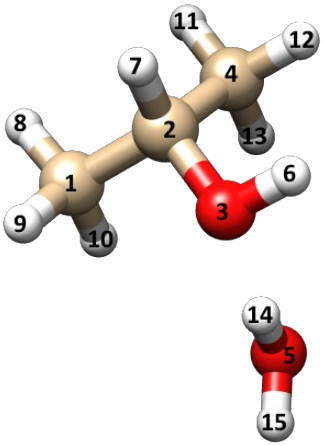

Table S4. MP2/6-311++G(d, p) geometry of the observed conformer of the *GAO* conformer of Isopropanol-water

bond lengths/Å		angles/°		dihedral angel/°	
C2C1	1.5213				
O3C2	1.4418	O3C2C1	110.3		
C4C2	1.5176	C4C2O3	106.3	C4C2O3C1	-122.4
O5O3	2.8602	O5O3C2	109.4	O5O3C2C1	178.3
H6O3	0.9629	H6O3C2	107.5	H6O3C2C1	-53.6
H7C2	1.0985	H7C2O3	108.6	H7C2O3O5	-61.6
H8C1	1.0941	H8C1C2	110.4	H8C1C2C4	-61.6
H9C1	1.0955	H9C1C2	111.1	H9C1C2C4	178.8
H10C1	1.0939	H10C1C2	109.9	H10C1C2C4	58.6

H11C4	1.0936	H11C4C2	110.0	H11C4C2C1	60.8
H12C4	1.0923	H12C4C2	109.8	H12C4C2C1	-58.8
H13C4	1.0943	H13C4C2	110.5	H13C4C2C1	-179.0
H14O5	0.9684	H14O5O3	5.6	H14O5O3C2	-164.8
H15O5	0.9589	H15O5O3	109.0	H15O5O3C2	-144.6