Electronic Supplementary Information for PCCP

Internal dynamics in complexes of water with organic molecules. Details of the internal motions in *tert*-butylalcohol-water

Luca Evangelisti, Walther Caminati

Supplementary Information

Content:

1) Table of transition frequencies
2) Sketch of the most stable conformer of TBA-W.
3) Table with MP2 optimized principal axes coordinates of the 2 conformers of TBA-W.
4) Table with MP2 optimized principal axes coordinates of the transition state of TBA-W.

Table 1. Experimental frequencies (MHz) of the measured lines of TBA-water

	HHH		DHH		DDH	
$J'K_a'K_c' \leftarrow J''K_a''K_c''$	0←0	1←1	0←0	1←1	0←0	1←1
2 0 2 ← 1 0 1	6863.4729	6861.3508				
2 1 2 ← 1 1 1	6848.2304					
2 1 1 ← 1 1 0	6878.6939					
3 0 3 ← 2 0 2	10294.9500	10291.7652	10243.5168	10243.1822	10115.2462	10115.0152
3 1 3 ← 2 1 2	10272.1959	10268.8582	10239.6896	10239.5245		
3 1 2 ← 2 1 1	10317.8884	10315.0678	10246.7996	10246.9121		
4 0 4 ← 3 0 3	13726.1174	13721.8732	13657.7391	13657.1670	13486.7310	13486.3087
4 1 4 ← 3 1 3	13695.9934	13691.5509	13652.5471	13652.6067	13483.710	13483.848
4 1 3 ← 3 1 2	13756.9140	13753.1540	13662.1936	13662.2961	13488.9735	13489.1020
4 2 2 ← 3 2 1	13726.6751	13723.0257				
4 2 3 ← 3 2 2	13726.6751	13722.4126				
4 3 2 ← 3 3 1	13725.4127	13722.4126				
5 0 5 ← 4 0 4	17156.8738	17151.5661			16857.9854	16857.2711
5 1 5 ← 4 1 4	17119.5624	17114.0172	17065.1045	17065.6188	16854.0771	16854.6777
5 1 4 ← 4 1 3	17195.7042	17191.0997	17077.1512	17077.7257	16860.6496	16861.2522
5 2 4 ← 4 2 3	17157.1765	17152.6348				
5 2 3 ← 4 2 2	17158.4032	17153.8670				
5 3 3 ← 4 3 2	17156.4994					
5 3 2 ← 4 3 1	17156.4994	17152.8129				
2 1 1 ← 1 0 1	9750.18090	9748.89690	9577.7577	9577.6747		
3 1 2 ← 2 0 2	13204.59930	13202.61530	12995.5598	12995.5157		
4 1 3 ← 3 0 3	16666.56030	16664.00260	16414.2305	16414.6174		

	HHD		HDH	HDD	DHD	$^{18}OH_2$
$J'K_a'K_c' \leftarrow J''K_a''K_c''$	0←0	1←1				
3 0 3 ← 2 0 2	9894.0193	9891.6661	10164.4757	9776.8773	9846.9699	9760.9858
3 1 3 ← 2 1 2	9871.9718	9869.6424	10144.0229	9756.7516	9842.0396	9740.4749
3 1 2 ← 2 1 1	9916.1217	9914.3023	10185.0260	9796.9819	9851.2110	9781.6255
4 0 4 ← 3 0 3	13191.5847	13188.4669	13552.2177	13035.4458	13129.0560	13014.2355
4 1 4 ← 3 1 3	13162.3841	13159.3291	13525.1226	13008.7813	13122.6585	12987.0553
4 1 3 ← 3 1 2	13221.2492	13218.8628	13579.7883	13062.3937	13134.753	13041.9133
4 2 2 ← 3 2 1			13552.5206			13014.1390
4 2 3 ← 3 2 2	13191.1558					13014.6181
5 0 5 ← 4 0 4	16488.7692	16484.9050	16939.5978	16293.6760	16410.944	16267.1308
5 1 5 ← 4 1 4	16452.5792		16906.0016	16260.6050	16403.2225	16233.4285
5 1 4 ← 4 1 3	16526.1571		16974.3292	16327.6150	16417.9239	16301.9914
5 2 4 ← 4 2 3	16488.5774		16939.5954	16293.1957		16267.3020
5 2 3 ← 4 2 2	16489.7526		16940.6540	16294.2047		16268.2659
5 3 3 ← 4 3 2						16266.6902
5 3 2 ← 4 3 1						16266.6902
2 1 1 ← 1 0 1			9672.8669			9480.9336
2 2 0 ← 1 1 0						15359.3639
2 2 1 ← 1 1 1						15373.0262
3 1 2 ← 2 0 2			13081.4268			12755.0824
4 1 3 ← 3 0 3			16496.7393			16036.0088

Figure 1. Sketch of the most stable conformer of TBA-W.

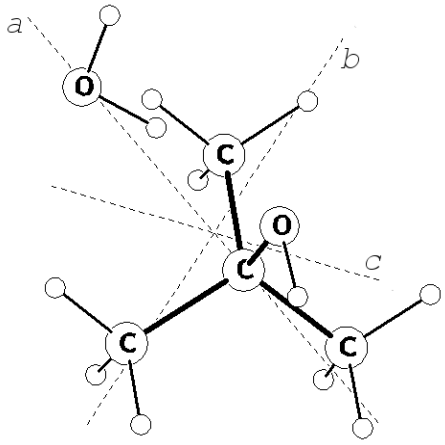
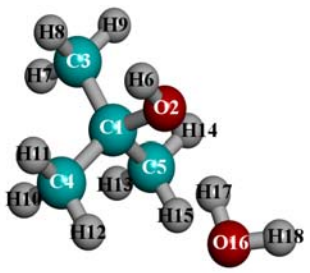


Table 2. MP2/6-311++G(d,p) principal axes coordinates of the 2 conformers of TBA-W.

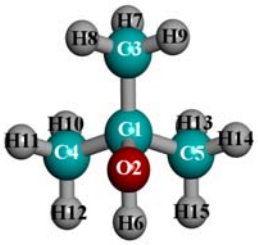
1) TBA-W conformer I:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	12	-0.712048	0.000833	-0.039746
2	16	0.216681	-0.141581	1.062016
3	12	-2.134846	-0.067883	0.504818
4	12	-0.460086	1.333349	-0.739455
5	12	-0.415948	-1.170618	-0.965224
6	1	0.019354	0.561148	1.691722
7	1	-2.860998	0.008609	-0.309852
8	1	-2.321606	0.757796	1.200943
9	1	-2.290290	-1.013026	1.031309
10	1	-1.128561	1.445544	-1.598171
11	1	-0.646388	2.168048	-0.054046
12	1	0.575101	1.387871	-1.085958
13	1	-1.092647	-1.148909	-1.824552
14	1	-0.555950	-2.113798	-0.430939
15	1	0.613804	-1.114610	-1.327329
16	16	2.843817	0.051893	-0.015221
17	1	2.002339	-0.088146	0.444413
18	1	3.441782	-0.566380	0.408871



2) TBA-W conformer II:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	12	-0.704724	0.271858	0.417565
2	16	0.172276	1.078310	-0.375066
3	12	-2.099311	0.831543	0.175982
4	12	-0.618104	-1.184693	-0.039377
5	12	-0.580653	-1.192384	-0.004857
6	1	1.070155	0.750147	-0.229419
7	1	-2.371147	0.748342	-0.880435
8	1	-2.052157	1.648457	-0.548640
9	1	-2.511883	1.220513	1.110400
10	1	-0.941824	-1.289552	-1.080163
11	1	0.043244	-1.263032	-0.907315
12	1	-0.214905	-1.809728	0.764231
13	1	0.435846	-1.563998	0.161447
14	1	0.191601	-1.293594	-0.773111
15	1	-1.530896	-1.549722	-0.415190
16	16	2.900632	0.103881	0.048455
17	1	3.257194	0.115032	0.940789
18	1	3.516052	0.690315	0.500365



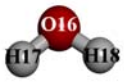


Table 2. MP2/6-311++G(d,p) principal axes coordinates of the transition state of TBA-W.

1) TBA-W transition state:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	12	-0.6998826	-0.0000000	-0.0427402
2	16	0.1949193	0.0000016	1.1007780
3	12	-2.1434040	0.0000005	0.4459534
4	12	-0.3947105	1.2581720	-0.8486553
5	12	-0.3947104	-1.2581740	-0.8486517
6	1	-0.3278900	0.0000027	1.9059310
7	1	-2.8317430	-0.0000005	-0.4030689
8	1	-2.3472240	0.8931528	1.0475780
9	1	-2.3472240	-0.8931500	1.0475810
10	1	-1.0427150	1.3143860	-1.7295380
11	1	-0.5650043	2.1470820	-0.2341030
12	1	0.6494731	1.2533100	-1.1716200
13	1	-1.0422280	-1.3140290	-1.7299150
14	1	-0.5656860	-2.1471050	-0.2343196
15	1	0.6496608	-1.2536530	-1.1710140
16	16	2.7937360	-0.0000001	-0.0320868
17	1	2.0368810	0.0000008	0.5697942
18	1	3.5556110	0.0000008	0.5503447