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Sizing the Ubbelhode effect: The rotational spectrum of tert-butylalcohol dimer

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Supplementary Information

Content:

1) Table of transition frequencies

2) Table with the ab initio cartesian coordinates of the atoms of $(TBA)_2$.

Table 1. Experimental frequencies, Obs.-Calc. values and estimated frequency errors (MHz) of the four isotopologues of $(TBA)_2$.

a) OH···OH

TRANSITION	Observed	Obs-Calc	Error
7, 1, 7 <- 6, 1, 6	7111.262	-0.001	0.003
7, 1, 6 <- 6, 1, 5	7115.585	0.000	0.003
7, 0, 7 <- 6, 0, 6	7113.424	0.001	0.003
7, 2, 6 <- 6, 2, 5	7113.405	-0.001	0.003
7, 2, 5 <- 6, 2, 4	7113.414	-0.001	0.003
8, 0, 8 <- 7, 0, 7	8129.577	-0.001	0.003
8, 1, 8 <- 7, 1, 7	8127.112	0.001	0.003
8, 1, 7 <- 7, 1, 6	8132.052	0.001	0.003
8, 2, 7 <- 7, 2, 6	8129.559	-0.002	0.003
8, 2, 6 <- 7, 2, 5	8129.577	0.002	0.003
8, 3, 6 <- 7, 3, 5	8129.526	-0.004	0.003
9, 0, 9 <- 8, 0, 8	9145.714	0.001	0.003
9, 1, 9 <- 8, 1, 8	9142.942	0.001	0.003
9, 1, 8 <- 8, 1, 7	9148.499	0.000	0.003
9, 2, 8 <- 8, 2, 7	9145.696	-0.002	0.003
9, 3, 7 <- 8, 3, 6	9145.657	-0.007	0.050
9, 4, 6 <- 8, 4, 5	9145.614	0.005	0.050
10, 0, 10 <- 9, 0, 9	10161.828	0.001	0.003
10, 2, 9 <- 9, 2, 8	10161.812	-0.003	0.003
10, 2, 8 <- 9, 2, 7	10161.844	0.002	0.003
10, 3, 7 <- 9, 3, 6	10161.780	0.001	0.003
10, 1, 10 <- 9, 1, 9	10158.751	0.000	0.003
10, 1, 9 <- 9, 1, 8	10164.928	0.001	0.003
11, 1, 11 <- 10, 1, 10	11174.538	0.001	0.003
11, 1, 10 <- 10, 1, 9	11181.331	0.000	0.003
11, 0, 11 <- 10, 0, 10	11177.918	0.001	0.003
11, 2, 9 <- 10, 2, 8	11177.947	0.003	0.003
11, 2, 10 <- 10, 2, 9	11177.907	-0.001	0.003
11, 3, 9 <- 10, 3, 8	11177.871	0.000	0.003
12, 0, 12 <- 11, 0, 11	12193.978	-0.002	0.003
12, 1, 12 <- 11, 1, 11	12190.299	0.000	0.003
12, 1, 11 <- 11, 1, 10	12197.712	0.002	0.003
12, 2, 11 <- 11, 2, 10	12193.978	0.001	0.003
12, 2, 10 <- 11, 2, 9	12194.023	0.000	0.003
12, 3, 10 <- 11, 3, 9	12193.938	-0.001	0.003
12, 4, 9 <- 11, 4, 8	12193.861	-0.001	0.003
12, 5, 8 <- 11, 5, 7	12193.766	-0.002	0.003
12, 6, 7 <- 11, 6, 6	12193.653	0.001	0.003
13, 1, 13 <- 12, 1, 12	13206.035	0.002	0.003
13, 1, 12 <- 12, 1, 11	13214.060	-0.002	0.003
13, 0, 13 <- 12, 0, 12	13210.016	0.002	0.003
13, 2, 11 <- 12, 2, 10	13210.075	-0.002	0.003
13, 2, 12 <- 12, 2, 11	13210.016	-0.002	0.003
13, 3, 10 <- 12, 3, 9	13209.978	-0.001	0.003
13, 4, 9 <- 12, 4, 8	13209.898	0.002	0.003
13, 5, 8 <- 12, 5, 7	13209.794	0.001	0.003
13, 6, 7 <- 12, 6, 6	13209.670	0.002	0.003
15, 0, 15 <- 14, 0, 14	15241.988	0.001	0.003
15, 2, 13 <- 14, 2, 12	15242.099	-0.001	0.003
15, 2, 14 <- 14, 2, 13	15242.014	0.004	0.003
15, 1, 15 <- 14, 1, 14	15237.409	0.000	0.003
15, 1, 14 <- 14, 1, 13	15246.673	0.000	0.003
15, 3, 12 <- 14, 3, 11	15241.969	-0.001	0.003
15, 4, 11 <- 14, 4, 10	15241.875	0.001	0.003
15, 5, 10 <- 14, 5, 9	15241.754	0.000	0.003
15, 6, 9 <- 14, 6, 8	15241.611	0.001	0.003

TRANSITION	Observed	Obs-Calc	Error
16, 2, 14 <- 15, 2, 13	16258.062	-0.002	0.003
16, 0, 16 <- 15, 0, 15	16257.917	-0.002	0.003
16, 2, 15 <- 15, 2, 14	16257.951	-0.004	0.003
16, 3, 14 <- 15, 3, 13	16257.917	0.000	0.003
16, 4, 13 <- 15, 4, 12	16257.812	-0.002	0.003
16, 1, 16 <- 15, 1, 15	16253.047	0.001	0.003
16, 1, 15 <- 15, 1, 14	16262.929	-0.001	0.003
16, 5, 12 <- 15, 5, 11	16257.685	0.000	0.003
17, 1, 17 <- 16, 1, 16	17268.648	0.001	0.003
17, 0, 17 <- 16, 0, 16	17273.813	-0.001	0.003
17, 2, 16 <- 16, 2, 15	17273.861	-0.003	0.003
17, 2, 15 <- 16, 2, 14	17273.996	0.001	0.003
17, 1, 16 <- 16, 1, 15	17279.151	0.003	0.003
17, 3, 14 <- 16, 3, 13	17273.831	0.003	0.003
17, 4, 13 <- 16, 4, 12	17273.717	0.000	0.003
17, 5, 12 <- 16, 5, 11	17273.578	-0.003	0.003
7, 1, 7 <- 6, 0, 6	8888.443	-0.002	0.003
6, 1, 5 <- 5, 0, 5	7887.403	0.002	0.003
7, 1, 6 <- 6, 0, 6	8905.734	-0.001	0.003
11, 4, 7 <- 10, 4, 6	11177.804	0.002	0.003
11, 5, 6 <- 10, 5, 5	11177.714	-0.001	0.003
10, 4, 7 <- 9, 4, 6	10161.717	0.001	0.003
10, 5, 6 <- 9, 5, 5	10161.635	-0.003	0.003
6, 2, 5 <- 5, 1, 4	11443.592	-0.002	0.003
6, 2, 4 <- 5, 1, 4	11443.606	0.002	0.003
6, 2, 4 <- 5, 1, 5	11452.868	0.002	0.003
6, 2, 5 <- 5, 1, 5	11452.854	-0.001	0.003
8, 2, 7 <- 7, 1, 7	13489.163	0.000	0.003
7, 2, 6 <- 6, 1, 6	12470.864	0.000	0.003
7, 2, 5 <- 6, 1, 5	12457.916	-0.001	0.003
9, 1, 8 <- 8, 0, 8	10943.285	0.001	0.003
8, 2, 6 <- 7, 1, 6	13471.905	-0.002	0.003
8, 1, 8 <- 7, 0, 7	9902.134	0.000	0.003
8, 1, 7 <- 7, 0, 7	9924.361	-0.002	0.003
4, 2, 2 <- 3, 1, 3	9417.718	-0.002	0.003
4, 2, 3 <- 3, 1, 3	9417.718	0.000	0.003
3, 2, 1 <- 2, 1, 1	8398.740	-0.003	0.003
3, 2, 2 <- 2, 1, 2	8400.592	-0.003	0.003
4, 2, 2 <- 3, 1, 2	9414.019	0.003	0.003
2, 2, 0 <- 1, 1, 0	7383.154	0.001	0.003
2, 2, 1 <- 1, 1, 1	7383.771	0.001	0.003
5, 2, 4 <- 4, 1, 3	10428.970	0.005	0.003
5, 2, 4 <- 4, 1, 4	10435.142	0.003	0.003
5, 2, 3 <- 4, 1, 3	10428.970	-0.001	0.003
5, 2, 3 <- 4, 1, 4	10435.142	-0.003	0.003
2, 2, 1 <- 1, 1, 0	7383.154	0.001	0.003
4, 2, 3 <- 3, 1, 2	9414.019	0.006	0.003
3, 2, 2 <- 2, 1, 1	8398.740	-0.002	0.003
3, 2, 1 <- 2, 1, 2	8400.592	-0.003	0.003
2, 2, 0 <- 1, 1, 1	7383.771	0.001	0.003

b) OH···OD

TRANSITION	Observed	Obs-Calc	Error
8, 0, 8 <- 7, 0, 7	8102.488	0.000	0.003
8, 1, 8 <- 7, 1, 7	8097.714	-0.002	0.003
8, 1, 7 <- 7, 1, 6	8107.328	0.000	0.003
8, 2, 7 <- 7, 2, 6	8102.513	0.006	0.003
8, 2, 6 <- 7, 2, 5	8102.557	-0.001	0.003
9, 0, 9 <- 8, 0, 8	9115.226	-0.001	0.003
9, 1, 9 <- 8, 1, 8	9109.869	0.000	0.003
9, 1, 8 <- 8, 1, 7	9120.682	-0.001	0.003
9, 2, 8 <- 8, 2, 7	9115.263	0.002	0.003

TRANSITION	Observed	Obs-Calc	Error
9, 2, 7 <- 8, 2, 6	9115.335	0.000	0.003
9, 3, 7 <- 8, 3, 6	9115.243	-0.003	0.003
9, 4, 6 <- 8, 4, 5	9115.194	0.004	0.003
10, 0, 10 <- 9, 0, 9	10127.943	0.002	0.003
10, 1, 10 <- 9, 1, 9	10122.002	-0.001	0.003
10, 1, 9 <- 9, 1, 8	10134.017	0.000	0.003
10, 2, 9 <- 9, 2, 8	10127.998	0.003	0.003
10, 2, 8 <- 9, 2, 7	10128.097	0.000	0.003
10, 3, 8 <- 9, 3, 7	10127.983	0.000	0.003
10, 4, 7 <- 9, 4, 6	10127.917	-0.003	0.003
11, 1, 11 <- 10, 1, 10	11134.114	0.002	0.003
11, 1, 10 <- 10, 1, 9	11147.327	-0.001	0.003
11, 0, 11 <- 10, 0, 10	11140.625	-0.001	0.003
11, 2, 9 <- 10, 2, 8	11140.845	0.004	0.003
11, 2, 10 <- 10, 2, 9	11140.703	-0.002	0.003
7, 1, 7 <- 6, 1, 6	7085.543	0.000	0.003
7, 1, 6 <- 6, 1, 5	7093.950	-0.003	0.003
7, 0, 7 <- 6, 0, 6	7089.729	0.002	0.003
7, 2, 6 <- 6, 2, 5	7089.739	0.005	0.003
7, 2, 5 <- 6, 2, 4	7089.763	-0.005	0.003
12, 1, 12 <- 11, 1, 11	12146.196	0.001	0.003
12, 1, 11 <- 11, 1, 10	12160.611	-0.002	0.003
12, 0, 12 <- 11, 0, 11	12153.285	0.004	0.003
12, 2, 11 <- 11, 2, 10	12153.385	-0.005	0.003
12, 2, 10 <- 11, 2, 9	12153.563	-0.004	0.003
13, 0, 13 <- 12, 0, 12	13165.903	0.002	0.003
13, 2, 11 <- 12, 2, 10	13166.275	0.003	0.003
13, 2, 12 <- 12, 2, 11	13166.043	-0.005	0.003
13, 3, 10 <- 12, 3, 9	13166.059	-0.001	0.003
13, 4, 9 <- 12, 4, 8	13165.972	0.000	0.003
15, 0, 15 <- 14, 0, 14	15191.029	0.001	0.003
15, 2, 14 <- 14, 2, 13	15191.271	0.002	0.003
15, 2, 13 <- 14, 2, 12	15191.612	-0.003	0.003
15, 3, 12 <- 14, 3, 11	15191.307	-0.002	0.003
15, 4, 11 <- 14, 4, 10	15191.206	0.003	0.003
6, 1, 5 <- 5, 0, 5	7843.480	-0.009	0.003
7, 1, 6 <- 6, 0, 6	8860.502	0.006	0.003
8, 1, 7 <- 7, 0, 7	9878.099	0.003	0.003

c) OD···OH

TRANSITION	Observed	Obs-Calc	Error
8, 0, 8 <- 7, 0, 7	8142.546	0.003	0.003
8, 1, 8 <- 7, 1, 7	8139.649	-0.002	0.003
8, 1, 7 <- 7, 1, 6	8145.452	0.001	0.003
9, 0, 9 <- 8, 0, 8	9160.298	-0.001	0.003
9, 1, 9 <- 8, 1, 8	9157.049	0.000	0.003
9, 1, 8 <- 8, 1, 7	9163.572	-0.002	0.003
9, 2, 8 <- 8, 2, 7	9160.289	-0.002	0.003
9, 2, 7 <- 8, 2, 6	9160.327	0.009	0.003
9, 3, 7 <- 8, 3, 6	9160.260	-0.001	0.003
10, 1, 10 <- 9, 1, 9	10174.426	-0.001	0.003
10, 1, 9 <- 9, 1, 8	10181.677	-0.001	0.003
10, 0, 10 <- 9, 0, 9	10178.034	0.002	0.003
10, 2, 9 <- 9, 2, 8	10178.028	-0.002	0.003
10, 2, 8 <- 9, 2, 7	10178.066	-0.001	0.003
10, 3, 7 <- 9, 3, 6	10178.005	0.007	0.003
10, 4, 6 <- 9, 4, 5	10177.943	0.005	0.003
11, 1, 11 <- 10, 1, 10	11191.780	-0.001	0.003
11, 1, 10 <- 10, 1, 9	11199.756	-0.002	0.003
11, 0, 11 <- 10, 0, 10	11195.744	0.002	0.003
11, 2, 9 <- 10, 2, 8	11195.796	0.001	0.003
11, 2, 10 <- 10, 2, 9	11195.744	-0.002	0.003

TRANSITION	Observed	Obs-Calc	Error
11, 3, 9 <- 10, 3, 8	11195.719	0.005	0.003
11, 4, 7 <- 10, 4, 6	11195.649	0.002	0.003
7, 0, 7 <- 6, 0, 6	7124.769	0.001	0.003
7, 2, 6 <- 6, 2, 5	7124.753	-0.003	0.003
7, 2, 5 <- 6, 2, 4	7124.769	0.001	0.003
7, 1, 7 <- 6, 1, 6	7122.237	0.003	0.003
7, 1, 6 <- 6, 1, 5	7127.311	0.002	0.003
8, 2, 7 <- 7, 2, 6	8142.534	0.001	0.003
8, 2, 6 <- 7, 2, 5	8142.546	-0.005	0.003
8, 3, 6 <- 7, 3, 5	8142.497	-0.007	0.003
8, 4, 5 <- 7, 4, 4	8142.456	0.000	0.003
12, 1, 12 <- 11, 1, 11	12209.107	-0.003	0.003
12, 1, 11 <- 11, 1, 10	12217.815	0.001	0.003
12, 0, 12 <- 11, 0, 11	12213.421	-0.003	0.003
12, 2, 11 <- 11, 2, 10	12213.440	0.002	0.003
12, 2, 10 <- 11, 2, 9	12213.502	0.001	0.003
12, 3, 10 <- 11, 3, 9	12213.402	-0.004	0.003
13, 1, 13 <- 12, 1, 12	13226.413	0.000	0.003
13, 1, 12 <- 12, 1, 11	13235.841	0.000	0.003
13, 0, 13 <- 12, 0, 12	13231.079	0.002	0.003
13, 2, 11 <- 12, 2, 10	13231.180	-0.002	0.003
13, 2, 12 <- 12, 2, 11	13231.100	-0.002	0.003
13, 3, 10 <- 12, 3, 9	13231.068	-0.003	0.003
13, 4, 9 <- 12, 4, 8	13230.987	-0.003	0.003
13, 5, 8 <- 12, 5, 7	13230.890	0.000	0.003
15, 0, 15 <- 14, 0, 14	15266.287	0.002	0.003
15, 2, 13 <- 14, 2, 12	15266.463	0.000	0.003
15, 2, 14 <- 14, 2, 13	15266.340	0.001	0.003
15, 3, 12 <- 14, 3, 11	15266.310	-0.003	0.003
15, 4, 11 <- 14, 4, 10	15266.215	-0.002	0.003
15, 5, 10 <- 14, 5, 9	15266.104	0.002	0.003
15, 1, 15 <- 14, 1, 14	15260.929	0.003	0.003
15, 1, 14 <- 14, 1, 13	15271.810	0.002	0.003
6, 1, 5 <- 5, 0, 5	7894.757	0.000	0.003
7, 1, 6 <- 6, 0, 6	8915.090	0.000	0.003
8, 1, 7 <- 7, 0, 7	9935.772	0.000	0.003

d) OD···OD

TRANSITION	Observed	Obs-Calc	Error
8, 0, 8 <- 7, 0, 7	8115.567	-0.001	0.003
8, 1, 8 <- 7, 1, 7	8110.711	0.003	0.003
8, 1, 7 <- 7, 1, 6	8120.492	-0.006	0.003
8, 2, 7 <- 7, 2, 6	8115.586	-0.003	0.003
8, 2, 6 <- 7, 2, 5	8115.644	0.001	0.003
9, 1, 9 <- 8, 1, 8	9124.486	-0.001	0.003
9, 1, 8 <- 8, 1, 7	9135.503	0.002	0.003
9, 0, 9 <- 8, 0, 8	9129.945	0.003	0.003
9, 2, 8 <- 8, 2, 7	9129.982	0.002	0.003
9, 2, 7 <- 8, 2, 6	9130.058	0.002	0.003
9, 3, 7 <- 8, 3, 6	9129.962	-0.005	0.003
10, 0, 10 <- 9, 0, 9	10144.292	0.001	0.003
10, 1, 10 <- 9, 1, 9	10138.246	0.002	0.003
10, 1, 9 <- 9, 1, 8	10150.482	-0.001	0.003
10, 2, 9 <- 9, 2, 8	10144.343	-0.006	0.003
10, 2, 8 <- 9, 2, 7	10144.453	-0.002	0.003
11, 1, 11 <- 10, 1, 10	11151.978	-0.001	0.003
11, 1, 10 <- 10, 1, 9	11165.444	0.004	0.003
11, 0, 11 <- 10, 0, 10	11158.609	-0.002	0.003
11, 2, 9 <- 10, 2, 8	11158.840	0.003	0.003
11, 2, 10 <- 10, 2, 9	11158.695	-0.001	0.003
12, 0, 12 <- 11, 0, 11	12172.901	0.001	0.003
12, 1, 12 <- 11, 1, 11	12165.687	0.000	0.003

12, 1, 11 <- 11, 1, 10	12180.373	0.000	0.003
12, 2, 11 <- 11, 2, 10	12173.020	0.002	0.003
12, 2, 10 <- 11, 2, 9	12173.203	0.002	0.003
12, 3, 10 <- 11, 3, 9	12173.024	-0.001	0.003
12, 4, 9 <- 11, 4, 8	12172.948	0.000	0.003
13, 1, 13 <- 12, 1, 12	13179.364	-0.004	0.003
13, 1, 12 <- 12, 1, 11	13195.279	0.002	0.003
13, 0, 13 <- 12, 0, 12	13187.156	0.000	0.003
13, 2, 11 <- 12, 2, 10	13187.547	0.001	0.003
13, 2, 12 <- 12, 2, 11	13187.312	0.000	0.003
13, 4, 9 <- 12, 4, 8	13187.246	0.000	0.003
13, 3, 10 <- 12, 3, 9	13187.330	0.000	0.003
7, 1, 7 <- 6, 1, 6	7096.910	0.000	0.003
7, 1, 6 <- 6, 1, 5	7105.480	0.003	0.003
7, 0, 7 <- 6, 0, 6	7101.173	0.001	0.003
7, 2, 6 <- 6, 2, 5	7101.184	0.003	0.003
7, 2, 5 <- 6, 2, 4	7101.212	-0.005	0.003
15, 1, 15 <- 14, 1, 14	15206.635	0.000	0.003
15, 1, 14 <- 14, 1, 13	15224.988	-0.003	0.003
15, 0, 15 <- 14, 0, 14	15215.556	0.002	0.003
15, 2, 14 <- 14, 2, 13	15215.810	0.001	0.003
15, 2, 13 <- 14, 2, 12	15216.170	0.002	0.003
15, 3, 12 <- 14, 3, 11	15215.860	0.004	0.003
15, 4, 11 <- 14, 4, 10	15215.758	0.005	0.003
17, 0, 17 <- 16, 0, 16	17243.783	0.000	0.003
17, 1, 17 <- 16, 1, 16	17233.764	0.002	0.003
17, 1, 16 <- 16, 1, 15	17254.562	-0.003	0.003
17, 2, 16 <- 16, 2, 15	17244.168	0.000	0.003
17, 2, 15 <- 16, 2, 14	17244.692	0.000	0.003
17, 3, 14 <- 16, 3, 13	17244.254	-0.002	0.003
17, 4, 13 <- 16, 4, 12	17244.133	0.001	0.003
16, 0, 16 <- 15, 0, 15	16229.691	0.000	0.003
16, 2, 15 <- 15, 2, 14	16230.007	-0.001	0.003
16, 2, 14 <- 15, 2, 13	16230.446	0.003	0.003
16, 3, 14 <- 15, 3, 13	16230.069	-0.002	0.003
16, 4, 13 <- 15, 4, 12	16229.956	-0.003	0.003
16, 5, 12 <- 15, 5, 11	16229.836	-0.001	0.003
16, 1, 16 <- 15, 1, 15	16220.216	-0.001	0.003
16, 1, 15 <- 15, 1, 14	16239.797	0.000	0.003
7, 1, 6 <- 6, 0, 6	8868.827	-0.002	0.003
6, 1, 5 <- 5, 0, 5	7850.109	0.002	0.003

Table 2. MP2/6-311++G(d,p) principal axes coordinates of $(TBA)_2$.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.456843	0.115006	0.957012
2	6	2.284824	-0.008350	-0.007153
3	8	1.164142	-0.395026	0.795019
4	6	2.557830	-1.085504	-1.058278
5	6	1.993790	1.332302	-0.683761
6	8	-1.216112	-0.553951	-0.777873
7	6	-2.284780	0.007282	0.024827
8	6	-3.584916	-0.051053	-0.770950
9	6	-2.397833	-0.778367	1.329512
10	6	-1.865998	1.446932	0.289303
11	1	-1.483224	-1.447823	-1.023211
12	1	0.403178	-0.473970	0.197140
13	1	-4.404452	0.399090	-0.201957
14	1	-3.472980	0.487321	-1.716435
15	1	-3.857854	-1.090373	-0.989809
16	1	-2.629168	1.954813	0.886706
17	1	-0.918546	1.471659	0.834632
18	1	-1.744339	1.983826	-0.656200
19	1	-3.177044	-0.350184	1.968404
20	1	-2.661588	-1.823285	1.127523
21	1	-1.446096	-0.755882	1.868275
22	1	3.435145	-0.832216	-1.663371
23	1	2.731974	-2.048248	-0.568246
24	1	1.696752	-1.185764	-1.728922
25	1	2.847007	1.660959	-1.287191
26	1	1.120535	1.243906	-1.339575
27	1	1.783876	2.094630	0.073016
28	1	4.365842	0.412434	0.424341
29	1	3.233323	0.865152	1.721456
30	1	3.634854	-0.843717	1.453176