Terpenoids: shape and non-covalent interactions. The rotational spectrum of *cis*-verbenol and its 1:1 water complex. Supporting Information

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Table 1: Experimental transition frequencies of *anti*, *cis*-verbenol.

J'	K_a'	K_c'	J	K_a	K_c	$\nu_{obs.}$ [MHz]	*obs.-calc.*
1	1	1	0	0	0	2218.7538	-0.0016
1	1	0	0	0	0	2494.8361	0.0027
2	0	2	1	1	1	3880.2612	-0.0018
2	1	2	1	0	1	4037.4797	-0.0013
2	2	0	1	1	1	5299.0085	-0.0018
2	2	1	1	1	0	4837.5387	0.0011
2	1	1	1	0	1	4865.7177	0.0030
2	2	1	1	1	1	5113.6199	0.0043
2	2	0	1	1	0	5022.9310	-0.0014
3	0	3	2	1	2	5769.7853	0.0000
3	1	2	2	2	1	6131.3115	-0.0017
3	1	3	2	0	2	5808.8801	-0.0004
3	2	2	2	1	1	6656.2562	-0.0041
3	2	1	2	1	2	8151.2424	-0.0029
3	3	1	2	2	0	7503.6354	-0.0043
3	3	0	2	2	1	7789.7107	-0.0051
3	1	2	2	0	2	7364.6856	0.0198
3	2	2	2	1	2	7484.4879	-0.0061
3	2	1	2	1	1	7323.0029	-0.0087
3	3	1	2	2	1	7689.0191	-0.0153
3	3	0	2	2	0	7604.3243	0.0032
4	1	3	4	0	4	2283.3060	0.0003
4	2	3	4	1	4	2321.4425	-0.0015
4	4	0	4	1	3	3551.7381	0.0096
4	0	4	3	1	3	7604.3790	-0.0044
4	1	3	3	2	2	8178.8076	-0.0006
4	2	2	3	3	1	8202.8667	0.0040
4	2	3	3	3	0	6712.4761	-0.0045
4	1	4	3	0	3	7611.0499	-0.0024
4	2	3	3	1	2	8370.8828	-0.0005
4	3	2	3	2	1	9338.9067	0.0007
4	3	1	3	2	2	10483.9705	0.0016
4	4	0	3	3	1	10325.9111	0.0001
4	1	3	3	0	3	9893.5271	0.0102
4	2	3	3	1	3	9926.6628	-0.0058
4	3	2	3	2	2	10005.6600	0.0027
4	3	1	3	2	1	9817.2178	0.0002
4	4	1	3	3	0	10179.1829	-0.0012
4	4	0	3	3	0	10225.2257	-0.0039
5	1	4	5	0	5	2967.6198	0.0025
5	2	4	5	1	5	2974.8519	-0.0059
5	2	3	5	1	4	2193.2313	-0.0001
5	3	3	5	2	4	2327.9066	-0.0012
5	5	1	5	4	2	2014.4249	-0.0019
5	4	1	5	1	4	4560.8818	-0.0154
5	5	0	5	2	3	4103.5712	-0.0051
5	0	5	4	1	4	9425.7072	-0.0007
5	1	4	4	2	3	10071.8847	0.0036
5	2	3	4	3	2	10477.2471	0.0042

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J'	K_a'	K_c'	J	K_a	K_c	$\nu_{obs.}$ [MHz]	*obs.-calc.*
5	3	2	4	4	1	10095.3058	0.0145
5	1	5	4	0	4	9426.6665	0.0080
5	2	4	4	1	3	10118.2135	0.0029
5	3	3	4	2	2	11017.4458	0.0076
6	1	5	6	0	6	3637.4787	0.0155
6	2	5	6	1	6	3638.6126	-0.0148
6	2	4	6	1	5	2921.8774	0.0000
6	3	4	6	2	5	2955.5353	-0.0008
6	3	3	6	2	4	2035.9904	0.0000
6	4	3	6	3	4	2364.6235	-0.0016
6	5	2	6	4	3	2139.2086	-0.0029
6	6	0	6	5	1	2245.4369	-0.0012
6	6	1	6	5	2	2397.3089	-0.0017
6	5	1	6	2	4	4697.6902	0.0009
6	0	6	5	1	5	11244.7234	-0.0073
6	1	5	5	2	4	11907.3399	0.0038
6	3	4	5	4	1	10310.5104	0.0078
6	1	6	5	0	5	11244.8238	-0.0298
6	2	5	5	1	4	11915.8703	0.0066
7	1	6	7	0	7	4303.8659	0.0070
7	2	6	7	1	7	4304.0229	-0.0051
7	2	5	7	1	6	3608.2099	0.0037
7	3	5	7	2	6	3614.8391	-0.0035
7	3	4	7	2	5	2830.1331	0.0005
7	4	4	7	3	5	2939.8436	-0.0010
7	5	3	7	4	4	2451.2990	0.0001
7	6	2	7	5	3	2420.3170	0.0003
7	7	0	7	6	1	2739.2991	0.0027
7	7	1	7	6	2	2811.6798	-0.0042
7	5	2	7	2	5	5998.3466	0.0155
7	6	1	7	3	4	5063.1045	-0.0068
8	1	7	8	0	8	4969.4049	0.0121
8	2	7	8	1	8	4969.4049	-0.0108
8	2	6	8	1	7	4280.2259	-0.0016
8	3	6	8	2	7	4281.3682	0.0044
8	3	5	8	2	6	3557.1242	-0.0004
8	4	5	8	3	6	3583.7972	-0.0006
8	4	4	8	3	5	2669.1755	-0.0006
8	5	4	8	4	5	2942.6438	-0.0001
8	6	3	8	5	4	2603.5489	0.0015
8	7	1	8	6	2	2433.9642	0.0058
8	7	2	8	6	3	2762.6661	-0.0011
8	8	0	8	7	1	3212.7738	0.0071
8	8	1	8	7	2	3244.1437	-0.0127
8	6	2	8	3	5	5935.0230	-0.0065
8	7	1	8	4	4	5699.8081	-0.0037
9	1	8	9	0	9	5634.6232	0.0041
9	2	8	9	1	9	5634.6232	0.0011
9	2	7	9	1	8	4948.2952	-0.0050
9	3	7	9	2	8	4948.4680	-0.0091
9	3	6	9	2	7	4244.4065	0.0061

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Table 1. *Continued from previous page*

J'	K_a'	K_c'	J	K_a	K_c	$\nu_{obs.}$ [MHz]	*obs.-calc.*
9	4	6	9	3	7	4249.7738	-0.0005
9	4	5	9	3	6	3466.9931	-0.0004
9	5	5	9	4	6	3550.5683	0.0000
9	5	4	9	4	5	2441.9692	-0.0005
9	6	4	9	5	5	2983.4001	-0.0006
9	7	2	9	6	3	2007.2468	0.0009
9	7	3	9	6	4	2828.7682	0.0000
9	8	1	9	7	2	2973.2086	0.0007
9	8	2	9	7	3	3151.5763	-0.0035
9	9	0	9	8	1	3672.8553	-0.0204
9	9	1	9	8	2	3685.6286	-0.0036
9	7	2	9	4	5	6092.7263	-0.0094
10	1	9	10	0	10	6299.6822	-0.0029
10	2	9	10	1	10	6299.6822	-0.0033
10	2	8	10	1	9	5615.0779	0.0137
10	3	8	10	2	9	5615.0779	-0.0121
10	3	7	10	2	8	4918.6428	0.0020
10	4	7	10	3	8	4919.6074	0.0077
10	4	6	10	3	7	4189.1781	0.0015
10	5	6	10	4	7	4209.0901	-0.0007
10	5	5	10	4	6	3313.6051	-0.0009
10	6	5	10	5	6	3526.4561	-0.0007
10	6	4	10	5	5	2202.9524	0.0002
10	7	4	10	6	5	3081.2813	0.0024
10	8	3	10	7	4	3124.6033	-0.0003
10	8	2	10	7	3	2548.0832	0.0038
10	9	2	10	8	3	3571.2112	-0.0029
10	9	1	10	8	2	3484.6854	0.0045
10	10	1	10	9	2	4130.9776	0.0142
10	10	0	10	9	1	4126.0089	-0.0062
10	8	2	10	5	5	6531.2066	-0.0113
11	1	10	11	0	11	6964.6460	-0.0026
11	2	10	11	1	11	6964.6460	-0.0026
11	2	9	11	1	10	6281.2159	-0.0022
11	3	9	11	2	10	6281.2159	-0.0057
11	3	8	11	2	9	5588.6936	-0.0016
11	4	8	11	3	9	5588.8545	0.0024
11	4	7	11	3	8	4877.2121	0.0084
11	5	7	11	4	8	4881.2678	-0.0041
11	5	6	11	4	7	4101.2828	-0.0003
11	6	6	11	5	7	4162.2322	-0.0006
11	6	5	11	5	6	3081.5840	-0.0011
11	7	5	11	6	6	3528.7378	0.0003
11	7	4	11	6	5	2042.2479	-0.0006
11	8	4	11	7	5	3249.9039	-0.0018
11	8	3	11	7	4	2112.0361	-0.0010
11	9	3	11	8	4	3480.2557	-0.0024
11	9	2	11	8	3	3128.8345	-0.0002
11	10	2	11	9	3	4008.3705	-0.0065
11	10	1	11	9	2	3969.6391	0.0005
11	11	1	11	10	2	4577.6681	0.0189

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Table 1. *Continued from previous page*

J'	K_a'	K_c'	J	K_a	K_c	$\nu_{obs.}$ [MHz]	*obs.-calc.*
11	11	0	11	10	1	4575.7910	0.0290
11	8	3	11	5	6	7235.8696	-0.0011
12	1	11	12	0	12	7629.5358	-0.0045
12	2	11	12	1	12	7629.5358	-0.0045
12	2	10	12	1	11	6947.0033	-0.0031
12	3	10	12	2	11	6947.0033	-0.0036
12	3	9	12	2	10	6257.0344	0.0076
12	4	9	12	3	10	6257.0344	-0.0165
12	4	8	12	3	9	5553.6852	0.0051
12	5	8	12	4	9	5554.4410	0.0135
12	5	7	12	4	8	4818.4538	0.0009
12	6	7	12	5	8	4832.7666	0.0008
12	6	6	12	5	7	3959.3216	0.0003
12	7	6	12	6	7	4117.2212	-0.0005
12	7	5	12	6	6	2795.6215	-0.0025
12	8	5	12	7	6	3577.5114	0.0010
12	8	4	12	7	5	2042.0336	-0.0028
12	9	4	12	8	5	3493.8920	-0.0005
12	9	3	12	8	4	2612.9942	0.0010
12	10	2	12	9	3	3690.9921	0.0011
12	9	3	12	6	6	7450.6477	-0.0059
13	1	12	13	0	13	8294.3693	-0.0095
13	2	11	13	1	12	7612.5443	-0.0032
13	3	11	13	2	12	7612.5443	-0.0032
13	3	10	13	2	11	6924.4169	-0.0011
13	4	10	13	3	11	6924.4169	-0.0046
13	4	9	13	3	10	6225.8491	0.0044
13	5	9	13	4	10	6225.9741	0.0025
13	5	8	13	4	9	5507.3799	0.0089
13	6	8	13	5	9	5510.3192	-0.0041
13	6	7	13	5	8	4732.3097	-0.0016
13	7	7	13	6	8	4775.4381	0.0014
13	7	6	13	6	7	3739.7230	-0.0025
13	8	6	13	7	7	4088.2151	0.0017
13	8	5	13	7	6	2533.1039	0.0001
13	9	5	13	8	6	3690.6982	0.0000
13	9	4	13	8	5	2248.6203	-0.0049
13	10	4	13	9	5	3808.1137	-0.0031
13	10	3	13	9	4	3211.2385	0.0019
13	11	3	13	10	4	4308.6561	-0.0048
13	11	2	13	10	3	4216.0782	0.0023
13	12	1	13	11	2	4896.6515	0.0080
14	2	12	14	1	13	8277.9119	0.0012
14	3	11	14	2	12	7591.1979	-0.0030
14	4	11	14	3	12	7591.1979	-0.0035
14	4	10	14	3	11	6895.9263	0.0065
14	5	10	14	4	11	6895.9263	-0.0137
14	5	9	14	4	10	6186.0631	-0.0035
14	6	9	14	5	10	6186.6242	0.0034
14	6	8	14	5	9	5445.4562	0.0065
14	7	8	14	6	9	5455.4674	-0.0011

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Table 1. *Continued from previous page*

J'	K_a'	K_c'	J	K_a	K_c	$\nu_{obs.}$ [MHz]	*obs.-calc.*
14	7	7	14	6	8	4601.4150	0.0003
14	8	7	14	7	8	4714.5522	0.0017
14	8	6	14	7	7	3440.4202	0.0006
14	9	6	14	8	7	4094.2143	0.0020
14	9	5	14	8	6	2392.9967	0.0023
14	10	5	14	9	6	3879.3259	0.0060
14	10	4	14	9	5	2664.1508	-0.0010
14	11	4	14	10	5	4179.8431	-0.0008
14	11	3	14	10	4	3824.4856	0.0040
14	12	3	14	11	4	4752.9459	-0.0040
14	12	2	14	11	3	4710.6761	-0.0093
14	14	1	14	13	2	5918.2292	0.0146
14	14	0	14	13	1	5918.1134	-0.0172
15	2	13	15	1	14	8943.1491	0.0082
15	4	12	15	3	13	8257.5517	-0.0049
15	4	11	15	3	12	7564.7308	-0.0023
15	5	11	15	4	12	7564.7308	-0.0053
15	5	10	15	4	11	6860.3692	0.0027
15	6	9	15	5	10	6135.4694	-0.0028
15	7	9	15	6	10	6137.5505	-0.0030
15	7	8	15	6	9	5360.2858	0.0013
15	8	8	15	7	9	5390.1249	-0.0083
15	8	7	15	7	8	4401.4506	0.0008
15	9	7	15	8	8	4660.9218	0.0013
15	9	6	15	8	7	3110.2385	-0.0039
15	10	6	15	9	7	4155.2592	-0.0003
15	10	5	15	9	6	2451.5701	0.0029
15	11	5	15	10	6	4144.8257	0.0009
15	11	4	15	10	5	3238.8341	0.0051
15	12	4	15	11	5	4592.8087	0.0009
15	12	3	15	11	4	4403.1027	0.0052
15	14	2	15	13	3	5803.3137	-0.0202
15	14	1	15	13	2	5802.3180	-0.0001
16	3	13	16	2	14	8923.6117	0.0138
16	4	12	16	3	13	8232.7007	0.0125
16	5	11	16	4	12	7532.2607	0.0017
16	6	11	16	5	12	7532.2607	-0.0143
16	6	10	16	5	11	6816.3317	-0.0056
16	7	10	16	6	11	6816.7479	0.0133
16	7	9	16	6	10	6070.6332	0.0005
16	8	9	16	7	10	6077.5025	-0.0081
16	8	8	16	7	9	5238.3986	-0.0011
16	9	8	16	8	9	5317.4278	0.0054
16	9	7	16	8	8	4113.7309	-0.0074
16	10	7	16	9	8	4631.0994	-0.0031
16	10	6	16	9	7	2845.5118	0.0011
16	11	6	16	10	7	4287.4522	-0.0007
16	11	5	16	10	6	2741.2686	-0.0065
16	12	5	16	11	6	4479.2815	0.0019
16	12	4	16	11	5	3884.8863	0.0032
16	13	4	16	12	5	5031.4818	-0.0017

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Table 1. *Continued from previous page*

J'	K_a'	K_c'	J	K_a	K_c	$\nu_{obs.}$ [MHz]	*obs.-calc.*
16	13	3	16	12	4	4938.2471	0.0068
16	14	3	16	13	4	5658.7898	-0.0133
16	14	2	16	13	3	5651.1747	0.0095
17	5	12	17	4	13	8202.6045	0.0105
17	6	11	17	5	12	7492.7584	0.0213
17	7	10	17	6	11	6761.9391	-0.0003
17	8	10	17	7	11	6763.3812	0.0052
17	8	9	17	7	10	5985.7289	0.0009
17	9	9	17	8	10	6006.0371	-0.0080
17	9	8	17	8	9	5058.4643	-0.0012
17	10	8	17	9	9	5245.0382	0.0009
17	10	7	17	9	8	3754.7292	0.0017
17	11	7	17	10	8	4645.1837	-0.0059
17	11	6	17	10	7	2747.4785	0.0080
17	12	6	17	11	7	4498.8173	-0.0014
17	12	5	17	11	6	3243.0338	0.0002
17	13	5	17	12	6	4868.2094	0.0061
17	13	4	17	12	5	4521.7259	0.0024
17	14	4	17	13	5	5483.8426	-0.0038
17	14	3	17	13	4	5440.7248	0.0030
18	7	11	18	6	12	7444.9392	0.0419
18	8	10	18	7	11	6694.3947	0.0000
18	9	10	18	8	11	6699.0398	-0.0067
18	9	9	18	8	10	5870.5027	-0.0086
18	10	9	18	9	10	5924.6599	-0.0026
18	10	8	18	9	9	4795.4955	-0.0008
18	11	8	18	10	9	5186.4088	0.0034
18	11	7	18	10	8	3397.7301	-0.0021
18	12	7	18	11	8	4722.5099	-0.0035
18	12	6	18	11	7	2881.7945	-0.0053
18	13	6	18	12	7	4787.5366	-0.0010
18	13	5	18	12	6	3884.2908	0.0007
18	14	4	18	13	5	5111.3870	-0.0010
18	14	5	18	13	6	5294.8462	-0.0037
18	15	3	18	14	4	5923.0189	-0.0084
19	8	11	19	7	12	7387.0920	-0.0087
19	9	11	19	8	12	7388.0798	0.0033
19	9	10	19	8	11	6609.2003	-0.0036
19	10	10	19	9	11	6622.8453	-0.0083
19	10	9	19	9	10	5707.7610	0.0139
19	11	9	19	10	10	5838.4372	0.0119
19	11	8	19	10	9	4440.7785	-0.0098
19	12	8	19	11	9	5160.0047	-0.0116
19	12	7	19	11	8	3152.4487	-0.0032
19	13	7	19	12	8	4876.8462	0.0032
19	13	6	19	12	7	3263.2673	-0.0135
19	14	6	19	13	7	5143.0380	0.0055
19	14	5	19	13	6	4567.7080	0.0072
19	15	4	19	14	5	5653.7541	0.0049
19	15	5	19	14	6	5744.1272	-0.0031
19	16	3	19	15	4	6393.7395	0.0310

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J'	K_a'	K_c'	J	K_a	K_c	$\nu_{obs.}$ [MHz]	*obs.-calc.*
19	16	4	19	15	5	6401.8088	-0.0096
20	9	11	20	8	12	7317.0551	0.0057
20	10	11	20	9	12	7320.1562	-0.0024
20	10	10	20	9	11	6498.6072	-0.0056
20	11	9	20	10	10	5472.8709	-0.0008
20	11	10	20	10	11	6535.1689	-0.0098
20	12	9	20	11	10	5757.5113	-0.0014
20	13	7	20	12	8	3116.1657	0.0183
20	14	7	20	13	8	5112.9626	0.0012
20	15	5	20	14	6	5220.2502	-0.0036
20	15	6	20	14	7	5549.3899	-0.0025
20	16	4	20	15	5	6162.6166	0.0019
20	16	5	20	15	6	6204.7918	-0.0141
20	17	3	20	16	4	6857.6739	-0.0047
21	10	11	21	9	12	7231.1961	-0.0047
21	11	11	21	10	12	7240.2675	-0.0077
21	11	10	21	10	11	6349.2620	-0.0091
21	12	10	21	11	11	6439.0002	-0.0016
21	12	9	21	11	10	5143.5628	-0.0020
21	13	9	21	12	10	5697.7575	0.0263
21	14	8	21	13	9	5283.6229	0.0077
21	15	7	21	14	8	5425.8240	-0.0009
21	16	6	21	15	7	5989.6868	-0.0004
21	16	5	21	15	6	5816.7045	0.0024
22	11	11	22	10	12	7123.6467	-0.0062
22	12	11	22	11	12	7148.0653	0.0066
22	12	10	22	11	11	6140.0967	-0.0087
22	13	10	22	12	11	6341.5214	0.0032
22	13	9	22	12	10	4726.5114	0.0020
22	14	9	22	13	10	5678.9961	-0.0009
22	15	8	22	14	9	5462.6385	0.0072
22	16	6	22	15	7	5257.7089	0.0048
22	16	7	22	15	8	5802.5002	0.0055
22	17	5	22	16	6	6364.1308	0.0025
22	17	6	22	16	7	6449.4372	-0.0124
23	11	12	23	10	13	7852.0985	-0.0064
23	12	11	23	11	12	6984.2590	-0.0004
23	13	11	23	12	12	7044.9374	-0.0026
23	13	10	23	12	11	5844.8459	-0.0148
23	14	10	23	13	11	6255.3603	-0.0009
23	15	9	23	14	10	5721.6734	-0.0015
23	16	8	23	15	9	5724.8692	0.0023
23	17	6	23	16	7	5919.4089	0.0009
23	18	6	23	17	7	6918.2910	-0.0186
23	18	5	23	17	6	6878.2183	0.0142
24	12	12	24	11	13	7746.4515	-0.0009
24	13	11	24	12	12	6796.1578	-0.0120
24	13	12	24	12	13	7762.5892	-0.0001
24	14	11	24	13	12	6935.6076	0.0044
24	14	10	24	13	11	5448.2479	-0.0030
24	15	10	24	14	11	6198.4036	-0.0036

Continue on next page

Table 1. *Continued from previous page*

J'	K_a'	K_c'	J	K_a	K_c	$\nu_{obs.}$ [MHz]	*obs.-calc.*
24	16	9	24	15	10	5841.8914	0.0018
24	17	8	24	16	9	6062.2070	-0.0037
24	17	7	24	16	8	5224.8004	0.0064
24	18	7	24	17	8	6679.5162	0.0043
24	18	6	24	17	7	6519.4333	-0.0062
24	19	5	24	18	6	7371.7699	0.0073
25	13	12	25	12	13	7614.2073	0.0057
25	14	12	25	13	13	7654.7424	-0.0048
25	14	11	25	13	12	6534.8350	-0.0039
25	15	11	25	14	12	6829.4911	-0.0114
25	15	10	25	14	11	4977.3977	0.0293
25	16	10	25	15	11	6191.4403	-0.0078
25	17	9	25	16	10	6047.5876	0.0128
25	18	8	25	17	9	6459.7146	-0.0006
26	14	12	26	13	13	7442.3517	-0.0049
26	17	10	26	16	11	6254.0349	-0.0075
26	18	9	26	17	10	6336.7204	-0.0040
26	19	7	26	18	8	6618.4943	0.0024
26	19	8	26	18	9	6899.7284	0.0039
26	20	7	26	19	8	7626.0656	-0.0098
27	15	12	27	14	13	7210.3636	0.0092
27	16	12	27	15	13	7416.7458	-0.0063
27	16	11	27	15	12	5713.0594	0.0157
27	18	10	27	17	11	6399.9264	-0.0021
27	19	9	27	18	10	6698.4191	0.0119
27	19	8	27	18	9	5913.6512	-0.0056
27	20	7	27	19	8	7219.8206	0.0066
28	17	12	28	16	13	7304.9668	-0.0014
28	18	11	28	17	12	6700.2695	-0.0087
29	18	12	29	17	13	7219.0538	-0.0063
29	19	11	29	18	12	6786.0546	0.0036

Table 2: Experimental transition frequencies and rotational constants for ^{13}C1 isotopologue of *anti*, *cis*-verbenol, and substitution coordinates of the substituted carbon atom.

J"	K_a"	K_c"	J'	K_a'	K_c'	$\nu_{obs.}$ [MHz]	obs.-calc.
2	0	2	1	1	1	3870.3378	0.0079
2	1	2	1	0	1	4028.9270	-0.0053
2	2	1	1	1	0	4826.1640	0.0177
2	2	0	1	1	1	5282.9800	-0.0055
3	0	3	2	1	2	5756.7900	-0.0012
3	1	3	2	0	2	5796.6457	-0.0076
3	2	2	2	1	1	6641.3061	-0.0028
3	3	1	2	2	0	7485.9612	-0.0033
4	0	4	3	1	3	7588.1230	0.0059
4	1	4	3	0	3	7594.9960	-0.0022

A_0 [MHz]	B_0 [MHz]	C_0 [MHz]	N_{lines}	*r.m.s.* [MHz]
1306.1883(28)	1181.4440(69)	907.5813(17)	10	0.0074

$\lvert a_s \rvert$ [Å]	$\lvert b_s \rvert$ [Å]	$\lvert c_s \rvert$ [Å]
0.8873(19)	0.5505(30)	0.8097(21)

Table 3: Experimental transition frequencies and rotational constants for ^{13}C2 isotopologue of *anti*, *cis*-verbenol, and substitution coordinates of the substituted carbon atom.

J"	K_a"	K_c"	J'	K_a'	K_c'	$\nu_{obs.}$ [MHz]	obs.-calc.
2	0	2	1	1	1	3871.4367	-0.0068
2	1	2	1	0	1	4016.9845	0.0048
2	2	1	1	1	0	4807.3430	-0.0044
2	2	0	1	1	1	5278.6245	0.0037
3	0	3	2	1	2	5748.4498	0.0025
3	1	3	2	0	2	5782.6518	-0.0006
3	2	2	2	1	1	6618.2500	0.0046
3	3	1	2	2	0	7453.8350	-0.0034
4	0	4	3	1	3	7573.3465	-0.0072
4	1	4	3	0	3	7578.8400	0.0062

A_0 [MHz]	B_0 [MHz]	C_0 [MHz]	N_{lines}	*r.m.s.* [MHz]
1300.6328(29)	1184.4752(68)	905.4490(17)	10	0.0048

$\lvert a_s \rvert$ [Å]	$\lvert b_s \rvert$ [Å]	$\lvert c_s \rvert$ [Å]
0.2671(62)	1.5278(11)	0.5274(32)

Table 4: Experimental transition frequencies and rotational constants for ^{13}C3 isotopologue of *anti*, *cis*-verbenol, and substitution coordinates of the substituted carbon atom.

J"	K_a"	K_c"	J'	K_a'	K_c'	$\nu_{obs.}$ [MHz]	obs.-calc.
2	0	2	1	1	1	3858.2802	-0.0080
2	1	2	1	0	1	4022.1190	-0.0263
2	2	1	1	1	0	4827.5830	0.0331
2	2	0	1	1	1	5283.5530	0.0004
3	0	3	2	1	2	5741.4345	0.0019
3	1	3	2	0	2	5783.4208	0.0019
3	2	2	2	1	1	6637.2659	-0.0055
3	3	1	2	2	0	7491.1111	-0.0129
4	0	4	3	1	3	7568.1317	0.0043
4	1	4	3	0	3	7575.5406	0.0070
A_0 [MHz]		B_0 [MHz]		C_0 [MHz]		N_{lines}	*r.m.s.* [MHz]
1307.5631(28)		1179.2483(69)		904.8608(17)		10	0.0102
$\|a_s\|$ [Å]		$\|b_s\|$ [Å]		$\|c_s\|$ [Å]			
1.4865(11)		0.7513(22)		0.083(20)			

Table 5: Experimental transition frequencies and rotational constants for ^{13}C4 isotopologue of *anti*, *cis*-verbenol, and substitution coordinates of the substituted carbon atom.

J"	K_a"	K_c"	J'	K_a'	K_c'	$\nu_{obs.}$ [MHz]	obs.-calc.
2	0	2	1	1	1	3860.6752	0.0129
2	1	2	1	0	1	4024.8957	0.0091
2	2	1	1	1	0	4830.4951	-0.0117
2	2	0	1	1	1	5286.1350	-0.0067
3	0	3	2	1	2	5745.2686	0.0019
3	1	3	2	0	2	5787.4115	-0.0072
3	2	2	2	1	1	6641.5530	0.0080
3	3	1	2	2	0	7495.6781	0.0067
4	0	4	3	1	3	7573.3465	0.0058
4	1	4	3	0	3	7580.7726	-0.0177

A_0 [MHz]	B_0 [MHz]	C_0 [MHz]	N_{lines}	*r.m.s.* [MHz]
1308.3292(28)	1179.7768(69)	905.5192(17)	10	0.0097

$\|a_s\|$ [Å]	$\|b_s\|$ [Å]	$\|c_s\|$ [Å]
1.4273(12)	0.5744(29)	0.024(68)

Table 6: Experimental transition frequencies and rotational constants for ^{13}C5 isotopologue of *anti*, *cis*-verbenol, and substitution coordinates of the substituted carbon atom.

J"	K_a"	K_c"	J'	K_a'	K_c'	$\nu_{obs.}$ [MHz]	obs.-calc.
2	0	2	1	1	1	3875.0248	0.0130
2	1	2	1	0	1	4024.2560	0.0076
2	2	1	1	1	0	4817.9610	0.0176
2	2	0	1	1	1	5286.2727	-0.0082
3	0	3	2	1	2	5756.3294	0.0117
3	1	3	2	0	2	5792.0400	0.0043
3	2	2	2	1	1	6631.6366	-0.0073
3	3	1	2	2	0	7471.2505	-0.0016
4	0	4	3	1	3	7584.5954	-0.0124
4	1	4	3	0	3	7590.4389	-0.0079

A_0 [MHz]	B_0 [MHz]	C_0 [MHz]	N_{lines}	*r.m.s.* [MHz]
1303.6977(28)	1185.0492(68)	906.8502(17)	10	0.0102

$\|a_s\|$ [Å]	$\|b_s\|$ [Å]	$\|c_s\|$ [Å]
i0.047(36)	1.2433(13)	0.3815(44)

Table 7: Experimental transition frequencies and rotational constants for ^{13}C6 isotopologue of *anti*, *cis*-verbenol, and substitution coordinates of the substituted carbon atom.

J"	K_a"	K_c"	J'	K_a'	K_c'	$\nu_{obs.}$ [MHz]	obs.-calc.
2	0	2	1	1	1	3870.3378	0.0006
2	1	2	1	0	1	4024.4790	0.0104
2	2	1	1	1	0	4804.1150	0.0026
2	2	0	1	1	1	5252.3820	-0.0012
3	0	3	2	1	2	5757.0167	0.0056
3	1	3	2	0	2	5795.5364	-0.0025
3	2	2	2	1	1	6621.4280	-0.0078
3	3	1	2	2	0	7447.3350	0.0022
4	0	4	3	1	3	7589.9688	-0.0011
4	1	4	3	0	3	7596.5770	-0.0032

A_0 [MHz]	B_0 [MHz]	C_0 [MHz]	N_{lines}	*r.m.s.* [MHz]
1298.4836(28)	1177.1075(69)	908.6617(17)	10	0.0048

$\lvert a_s \rvert$ [Å]	$\lvert b_s \rvert$ [Å]	$\lvert c_s \rvert$ [Å]
0.3167(53)	0.5667(29)	1.7130(98)

Table 8: Experimental transition frequencies and rotational constants for ^{13}C7 isotopologue of *anti*, *cis*-verbenol, and substitution coordinates of the substituted carbon atom.

J"	K_a"	K_c"	J'	K_a'	K_c'	$\nu_{obs.}$ [MHz]	obs.-calc.
2	0	2	1	1	1	3868.8743	0.0051
2	1	2	1	0	1	4029.5124	-0.0156
2	2	1	1	1	0	4831.8297	-0.0051
2	2	0	1	1	1	5289.9901	-0.0035
3	0	3	2	1	2	5755.2141	0.0017
3	1	3	2	0	2	5795.8165	-0.0029
3	2	2	2	1	1	6646.0290	0.0069
3	3	1	2	2	0	7496.2288	0.0040
4	0	4	3	1	3	7585.8463	-0.0044
4	1	4	3	0	3	7592.9112	0.0066

A_0 [MHz]	B_0 [MHz]	C_0 [MHz]	N_{lines}	*r.m.s.* [MHz]
1308.2470(28)	1182.0453(69)	907.0937(17)	10	0.0067

$\lvert a_s \rvert$ [Å]	$\lvert b_s \rvert$ [Å]	$\lvert c_s \rvert$ [Å]
1.0653(16)	0.5095(33)	0.2951(57)

Table 9: Experimental transition frequencies and rotational constants for ^{13}C8 isotopologue of *anti*, *cis*-verbenol, and substitution coordinates of the substituted carbon atom.

J"	K_a"	K_c"	J'	K_a'	K_c'	$\nu_{obs.}$ [MHz]	obs.-calc.
2	0	2	1	1	1	3812.3131	-0.0019
2	1	2	1	0	1	3989.0766	0.0032
2	2	1	1	1	0	4803.4072	0.0047
2	2	0	1	1	1		
3	0	3	2	1	2	5681.6867	0.0051
3	1	3	2	0	2	5729.5688	-0.0016
3	2	2	2	1	1	6594.3610	0.0040
3	3	1	2	2	0	7459.1383	-0.0053
4	0	4	3	1	3	7491.8180	-0.0022
4	1	4	3	0	3	7500.8113	-0.0025
A_0 [MHz]		B_0 [MHz]		C_0 [MHz]		N_{lines}	*r.m.s.* [MHz]
1302.6418(33)		1166.013(14)		895.4772(24)		9	0.0036
$\lvert a_s \rvert$ [Å]		$\lvert b_s \rvert$ [Å]		$\lvert c_s \rvert$ [Å]			
2.5639(79)		1.4349(15)		0.5068(41)			

Table 10: Experimental transition frequencies and rotational constants for ^{13}C9 isotopologue of *anti*, *cis*-verbenol, and substitution coordinates of the substituted carbon atom.

J"	K_a"	K_c"	J'	K_a'	K_c'	$\nu_{obs.}$ [MHz]	obs.-calc.
2	0	2	1	1	1	3822.6968	-0.0026
2	1	2	1	0	1	3997.3013	0.0040
2	2	1	1	1	0	4811.2530	0.0100
2	2	0	1	1	1	5258.6485	0.0014
3	0	3	2	1	2	5695.4647	0.0010
3	1	3	2	0	2	5742.2835	-0.0055
3	2	2	2	1	1	6606.3980	-0.0072
3	3	1	2	2	0	7470.5182	-0.0032
4	0	4	3	1	3	7509.4080	-0.0080
4	1	4	3	0	3	7518.1227	0.0129

A_0 [MHz]	B_0 [MHz]	C_0 [MHz]	N_{lines}	*r.m.s.* [MHz]
1304.5540(28)	1169.2691(69)	897.5811(17)	10	0.0067

$\|a_s\|$ [Å]	$\|b_s\|$ [Å]	$\|c_s\|$ [Å]
2.3858(7)	1.2753(14)	0.131(13)

Table 11: Experimental transition frequencies and rotational constants for ^{13}C10 isotopologue of *anti*, *cis*-verbenol, and substitution coordinates of the substituted carbon atom.

J"	K_a"	K_c"	J'	K_a'	K_c'	$\nu_{obs.}$ [MHz]	obs.-calc.
2	0	2	1	1	1	3863.3500	-0.0073
2	1	2	1	0	1	4022.2648	0.0000
2	2	1	1	1	0	4803.9145	0.0070
2	2	0	1	1	1	5246.6353	0.0036
3	0	3	2	1	2	5750.2932	0.0016
3	1	3	2	0	2	5790.9836	-0.0005
3	2	2	2	1	1	6619.6342	0.0050
3	3	1	2	2	0	7448.2650	-0.0094
4	0	4	3	1	3	7582.4598	-0.0054
4	1	4	3	0	3	7589.6443	0.0062

A_0 [MHz]	B_0 [MHz]	C_0 [MHz]	N_{lines}	*r.m.s.* [MHz]
1298.6822(28)	1174.2257(69)	907.8608(17)	10	0.0054

$\|a_s\|$ [Å]	$\|b_s\|$ [Å]	$\|c_s\|$ [Å]
0.9435(18)	0.124(13)	1.7875(9)

Table 12: Experimental transition frequencies and rotational constants for OD isotopologue of *anti*, *cis*-verbenol, and substitution coordinates of the substituted carbon atom.

J"	K_a"	K_c"	J'	K_a'	K_c'	$\nu_{obs.}$ [MHz]	obs.-calc.
2	1	2	1	0	1	3992.0140	0.0057
2	2	0	1	1	1	5243.6980	-0.0144
2	2	1	1	1	0	4765.6590	0.0043
3	0	3	2	1	2	5722.9710	-0.0126
3	1	3	2	0	2	5752.0900	-0.0042
4	1	3	3	2	2	8129.0470	0.0173
4	2	3	3	1	2	8273.3200	0.0222
4	3	2	3	2	1	9199.7370	0.0036
4	4	1	3	3	0	10015.6690	-0.0057
5	0	5	4	1	4	9341.9030	-0.0070
5	1	5	4	0	4	9342.4440	-0.0066
5	1	4	4	2	3	9988.2820	-0.0018
5	2	4	4	1	3	10018.6280	-0.0028

A_0 [MHz]	B_0 [MHz]	C_0 [MHz]	N_{lines}	*r.m.s.* [MHz]
1288.1195(20)	1181.1713(47)	901.2963(13)	13	0.0102

$\|a_s\|$ [Å]	$\|b_s\|$ [Å]	$\|c_s\|$ [Å]
0.2483(63)	2.2041(7)	1.2359(13)

Table 13: Comparison between the theoretical MP2/6-311++G(d,p) equilibrium coordinates and experimental Kraitchman's substitution coordinates of *anti*, *cis*-verbenol.

	r_e			r_s		
	a_e [Å]	b_e [Å]	c_e [Å]	$\|a_s\|$ [Å]	$\|b_s\|$ [Å]	$\|c_s\|$ [Å]
C1	-0.8928	0.5485	-0.8126	0.8873(19)	0.5505(30)	0.8097(21)
C2	0.2415	1.5396	-0.5307	0.2671(62)	1.5278(11)	0.5274(32)
C3	1.4697	0.7921	-0.0645	1.4865(11)	0.7513(22)	0.083(20)
C4	1.4413	-0.5553	0.0292	1.4273(12)	0.5744(29)	0.024(68)
C5	0.1555	-1.2408	-0.3789	i0.047(36)	1.2433(13)	0.3815(44)
C6	-0.3093	-0.5789	-1.7098	0.3167(53)	0.5667(29)	1.7130(98)
C7	-1.0579	-0.5286	0.3124	1.0653(16)	0.5095(33)	0.2951(57)
C8	2.5908	-1.3922	0.5088	2.5639(79)	1.4349(15)	0.5068(41)
C9	-2.3608	-1.3131	0.1346	2.3858(7)	1.2753(14)	0.131(13)
C10	-0.9394	-0.1487	1.7866	0.9435(18)	0.123(13)	1.7875(9)
H12	-0.2293	2.1698	1.2456	0.2483(63)	2.2041(7)	1.2359(13)

Table 14: Theoretical MP2/6-311++G(d,p) equilibrium structure of the three conformers of *cis*-verbenol in the principal axis system of coordinates.

	anti			*gauche'*			*gauche*		
	a_e [Å]	b_e [Å]	c_e [Å]	a_e [Å]	b_e [Å]	c_e [Å]	a_e [Å]	b_e [Å]	c_e [Å]
C1	-0.8928	0.5485	-0.8126	-0.9180	0.4904	-0.8230	0.9017	-0.5326	-0.8186
C2	0.2415	1.5396	-0.5307	0.1552	1.5406	-0.5529	-0.2323	-1.5270	-0.5520
C3	1.4697	0.7921	-0.0645	1.4252	0.8716	-0.0784	-1.4602	-0.7973	-0.0722
C4	1.4413	-0.5553	0.0292	1.4755	-0.4730	0.0304	-1.4417	0.5485	0.0257
C5	0.1555	-1.2408	-0.3789	0.2298	-1.2318	-0.3679	-0.1573	1.2427	-0.3699
C6	-0.3093	-0.5789	-1.7098	-0.2723	-0.6131	-1.7060	0.3183	0.6012	-1.7070
C7	-1.0579	-0.5286	0.3124	-1.0188	-0.5749	0.3195	1.0539	0.5252	0.3233
C8	2.5908	-1.3922	0.5088	2.6681	-1.2360	0.5268	-2.5960	1.3732	0.5136
C9	-2.3608	-1.3131	0.1346	-2.2746	-1.4358	0.1548	2.3498	1.3257	0.1645
C10	-0.9394	-0.1487	1.7866	-0.9177	-0.1557	1.7816	0.9256	0.1087	1.7843
O11	-0.1413	2.5788	0.3793	-0.3715	2.4675	0.4114	0.1088	-2.5092	0.4378
H12	-0.2293	2.1698	1.2456	0.3002	3.1427	0.5536	0.7740	-3.0834	0.0437
H13	0.4882	-0.2925	-2.4028	0.5057	-0.2942	-2.4072	-0.4725	0.3196	-2.4099
H14	-1.7944	1.0804	-1.1379	-1.8473	0.9677	-1.1546	1.8113	-1.0517	-1.1510
H15	0.4641	2.0782	-1.4611	0.3490	2.0833	-1.4930	-0.4661	-2.0446	-1.4979
H16	2.3559	1.3687	0.1983	2.2837	1.4941	0.1776	-2.3357	-1.3867	0.1949
H17	3.4600	-0.7749	0.7539	3.5022	-0.5680	0.7617	-3.4612	0.7478	0.7526
H18	2.3019	-1.9616	1.4013	2.4064	-1.8008	1.4303	-2.3088	1.9324	1.4128
H19	2.8825	-2.1213	-0.2569	3.0008	-1.9638	-0.2232	-2.8927	2.1098	-0.2431
H20	-1.0758	-1.1458	-2.2406	-1.0096	-1.2277	-2.2245	1.0865	1.1783	-2.2242
H21	0.2154	-2.3337	-0.3143	0.3496	-2.3189	-0.2907	-0.2206	2.3346	-0.2930
H22	-3.2102	-0.7011	0.4615	-3.1577	-0.8628	0.4619	3.2064	0.7077	0.4595
H23	-2.5432	-1.6132	-0.8999	-2.4348	-1.7764	-0.8713	2.5215	1.6736	-0.8573
H24	-2.3406	-2.2189	0.7526	-2.2072	-2.3205	0.7993	2.3279	2.2033	0.8218
H25	-1.7460	0.5379	2.0725	-1.7771	0.4671	2.0530	1.7780	-0.5174	2.0715
H26	-1.0406	-1.0477	2.4077	-0.9296	-1.0511	2.4172	0.9366	1.0053	2.4182
H27	0.0234	0.3079	2.0313	-0.0155	0.4167	1.9953	0.0167	-0.4570	1.9869

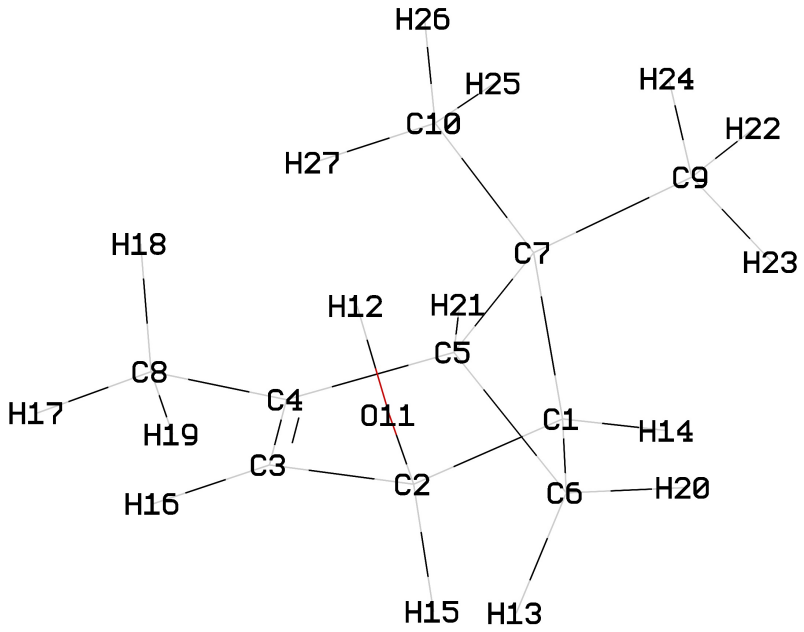

Figure 1: Sketch and numbering of the atoms of the *anti* conformer of *cis*-verbenol, as given in Table 14.

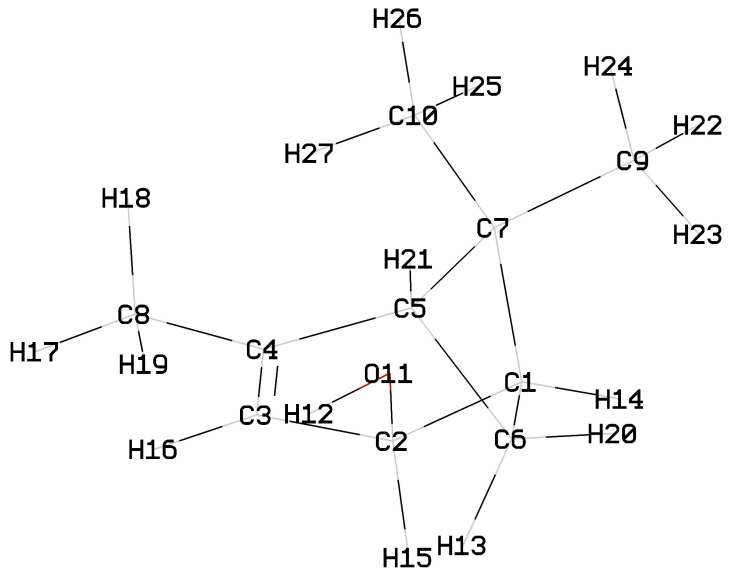

Figure 2: Sketch and numbering of the atoms of the *gauche*′ conformer of *cis*-verbenol, as given in Table 14.

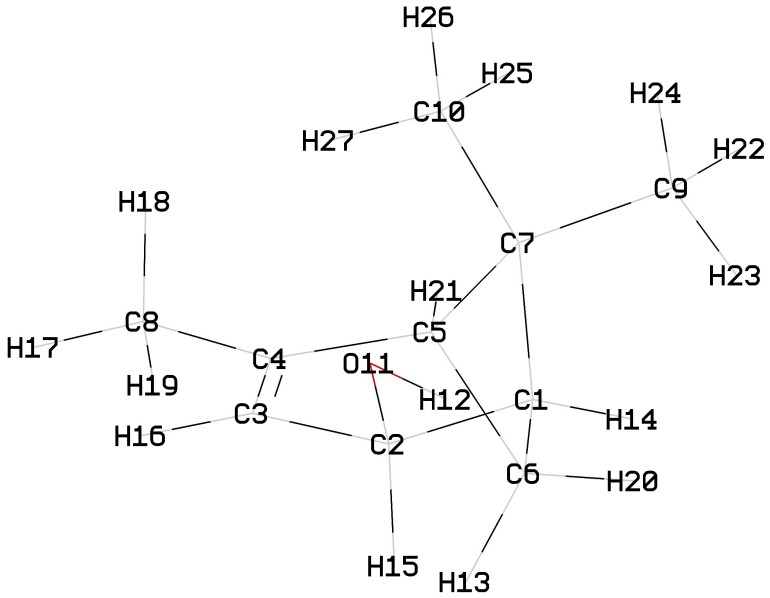

Figure 3: Sketch and numbering of the atoms of the *gauche* conformer of *cis*-verbenol, as given in Table 14.

Table 15: Experimental transition frequencies of *anti*, s−*cis*-verbenol-water molecular complex.

J"	K_a"	K_c"	J'	K_a'	K_c'	$\nu_{obs.}$ [MHz]	obs.-calc.
3	0	3	2	0	2	3949.243	-0.002
3	1	3	2	1	2	3826.772	0.000
3	1	2	2	1	1	4206.793	0.005
4	0	4	3	0	3	5189.976	-0.002
4	1	4	3	1	3	5082.313	0.004
4	1	3	3	1	2	5578.867	0.006
5	0	5	4	0	4	6402.210	-0.004
5	1	5	4	1	4	6325.979	0.001
5	1	4	4	1	3	6919.015	-0.001
5	2	4	4	2	3	6670.061	-0.001
5	2	3	4	2	2	6983.217	0.011
5	3	3	4	3	2	6769.215	-0.011
5	3	2	4	3	1	6813.231	-0.011
6	0	6	5	0	5	7605.594	-0.002
6	1	6	5	1	5	7559.616	0.009
6	2	5	5	2	4	7966.963	-0.001

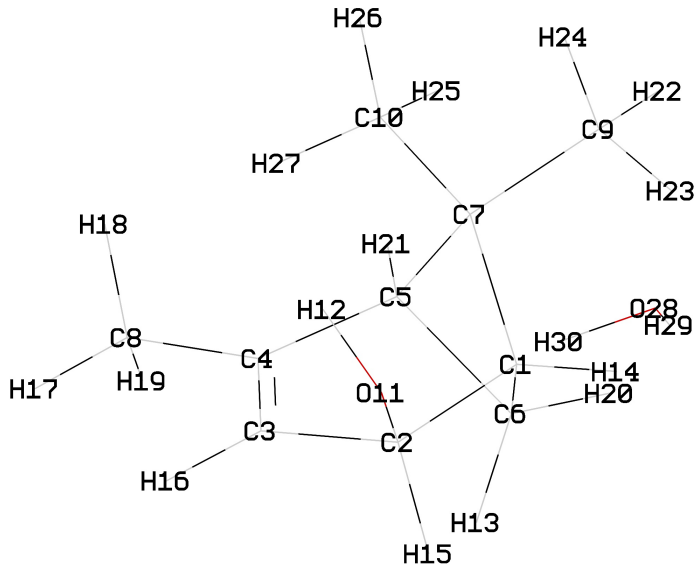

Figure 4: Sketch and numbering of the atoms of the observed water complex of *cis*-verbenol (AD1), as given in Table 16.

Table 16: Theoretical MP2/6-311++G(d,p) equilibrium structure of the three conformers of *anti*,*cis*-verbenol$\cdots$water complex in the principal axis system of coordinates.

	AA			AD1			AD2		
	a_e [Å]	b_e [Å]	c_e [Å]	a_e [Å]	b_e [Å]	c_e [Å]	a_e [Å]	b_e [Å]	c_e [Å]
C1	0.7238	0.9217	0.9771	-0.5696	0.2426	0.8331	0.5306	1.0111	0.8406
C2	-0.4994	0.1283	1.4529	-0.4008	-1.2544	0.5634	-0.9104	0.5394	0.6414
C3	-0.5301	-1.2179	0.7676	1.0009	-1.5438	0.0880	-0.9322	-0.8890	0.1515
C4	0.4540	-1.5571	-0.0932	1.8838	-0.5288	-0.0408	0.2338	-1.5486	-0.0225
C5	1.5623	-0.5471	-0.2967	1.4037	0.8509	0.3525	1.5034	-0.7970	0.3162
C6	1.9579	-0.0142	1.1119	0.6403	0.6909	1.7007	1.2568	-0.0802	1.6767
C7	0.9340	0.8633	-0.5717	0.0131	1.1325	-0.3153	1.4681	0.6201	-0.3527
C8	0.4984	-2.8497	-0.8542	3.2903	-0.6961	-0.5348	0.3350	-2.9606	-0.5198
C9	1.9863	1.8811	-1.0207	-0.4292	2.5887	-0.1456	2.8158	1.3392	-0.2486
C10	-0.2545	0.9638	-1.5227	-0.1903	0.7551	-1.7810	0.9878	0.7338	-1.7980
O11	-1.7211	0.8523	1.2942	-1.3868	-1.7581	-0.3682	-1.6610	1.4187	-0.2256
H12	-2.1179	0.6069	0.4475	-1.0544	-1.5678	-1.2524	-1.2517	1.3665	-1.0959
H13	1.9312	-0.7488	1.9234	1.0517	-0.0472	2.3967	0.6486	-0.6301	2.4017
H14	0.7448	1.9098	1.4518	-1.5845	0.4671	1.1758	0.5543	2.0523	1.1828
H15	-0.3954	-0.0145	2.5385	-0.6121	-1.8038	1.4898	-1.4411	0.6152	1.5988
H16	-1.3652	-1.8861	0.9758	1.2672	-2.5728	-0.1516	-1.8995	-1.3482	-0.0466
H17	-0.3527	-3.4900	-0.6039	3.5119	-1.7414	-0.7697	-0.6539	-3.3887	-0.7071
H18	0.4847	-2.6557	-1.9343	3.4505	-0.0912	-1.4361	0.9160	-2.9971	-1.4500
H19	1.4250	-3.3953	-0.6371	4.0061	-0.3454	0.2186	0.8582	-3.5893	0.2109
H20	2.9078	0.5228	1.1295	0.4632	1.6328	2.2218	2.1666	0.2845	2.1561
H21	2.3454	-0.9044	-0.9763	2.1853	1.6146	0.2627	2.4067	-1.4041	0.1853
H22	1.5500	2.8876	-1.0216	-1.4780	2.6887	-0.4483	3.2325	1.3254	0.7612
H23	2.8695	1.9000	-0.3775	-0.3423	2.9464	0.8830	2.7028	2.3874	-0.5510
H24	2.3149	1.6557	-2.0428	0.1757	3.2425	-0.7856	3.5432	0.8708	-0.9225
H25	-0.7468	1.9372	-1.4079	-1.2593	0.7488	-2.0255	0.8012	1.7834	-2.0601
H26	0.0983	0.8845	-2.5595	0.2919	1.5029	-2.4232	1.7685	0.3661	-2.4755
H27	-0.9944	0.1791	-1.3565	0.2440	-0.2162	-2.0354	0.0868	0.1458	-1.9944
O28	-3.5692	0.1939	-0.8488	-3.7657	-0.2266	0.0141	-4.1944	0.1502	-0.1144
H29	-4.3967	0.3070	-0.3723	-4.5775	-0.7386	-0.1302	-3.4188	0.7274	-0.1883
H30	-3.6951	0.6997	-1.6564	-3.0544	-0.8647	-0.1466	-4.8764	0.7256	0.2375

Table 17: Theoretical MP2/6-311++G(d,p) equilibrium structure of the two conformers of *gauche*, *cis*-verbenol· · ·water complex in the principal axis system of coordinates.

	GA			GD		
	a_e [Å]	b_e [Å]	c_e [Å]	a_e [Å]	b_e [Å]	c_e [Å]
C1	0.4905	-0.5431	0.6777	-0.8056	-0.9547	0.8936
C2	0.7826	0.9220	0.3313	0.6350	-0.5111	1.1523
C3	-0.5037	1.6410	0.0103	0.8618	0.8789	0.6181
C4	-1.6784	0.9815	0.0855	-0.1654	1.5456	0.0504
C5	-1.6175	-0.4693	0.5100	-1.4967	0.8303	-0.0075
C6	-0.6529	-0.5515	1.7299	-1.7323	0.1892	1.3923
C7	-0.5108	-1.2063	-0.3236	-1.2808	-0.6228	-0.5592
C8	-3.0104	1.5896	-0.2428	-0.0506	2.9237	-0.5304
C9	-0.5715	-2.7233	-0.1225	-2.6110	-1.3131	-0.8738
C10	-0.4066	-0.9265	-1.8187	-0.3442	-0.8284	-1.7449
O11	1.6662	1.0638	-0.7817	1.5952	-1.3910	0.5254
H12	2.5373	0.7721	-0.4775	1.6235	-2.2043	1.0410
H13	-0.6894	0.2940	2.4247	-1.3806	0.7712	2.2502
H14	1.4208	-1.0826	0.8984	-0.9778	-1.9751	1.2623
H15	1.2450	1.3912	1.2175	0.8192	-0.5216	2.2386
H16	-0.4443	2.6844	-0.2957	1.8582	1.3083	0.7021
H17	-2.9103	2.6429	-0.5214	0.9599	3.3246	-0.4105
H18	-3.4793	1.0504	-1.0756	-0.2961	2.9049	-1.5997
H19	-3.6924	1.5160	0.6134	-0.7610	3.6067	-0.0487
H20	-0.7211	-1.4897	2.2836	-2.7595	-0.1375	1.5612
H21	-2.6074	-0.9367	0.5770	-2.2898	1.4388	-0.4574
H22	0.3336	-3.1884	-0.5323	-2.4415	-2.3817	-1.0532
H23	-0.6552	-3.0174	0.9270	-3.3474	-1.2191	-0.0717
H24	-1.4334	-3.1370	-0.6603	-3.0461	-0.8852	-1.7849
H25	0.5024	-1.3869	-2.2229	-0.1461	-1.8966	-1.8890
H26	-1.2691	-1.3728	-2.3321	-0.8242	-0.4474	-2.6560
H27	-0.3670	0.1377	-2.0490	0.6139	-0.3245	-1.6181
O28	4.2572	0.2004	0.2234	3.9855	-0.2388	-0.5511
H29	4.7207	-0.5053	-0.2357	3.1877	-0.6677	-0.2091
H30	4.9289	0.8755	0.3532	3.8667	-0.2787	-1.5021

Table 18: Theoretical MP2/6-311++G(d,p) equilibrium structure of the two conformers of *gauche′*, *cis*-verbenol· · ·water complex in the principal axis system of coordinates.

	G'A			G'D		
	a_e [Å]	b_e [Å]	c_e [Å]	a_e [Å]	b_e [Å]	c_e [Å]
C1	0.5731	-1.0035	-0.8652	0.5221	-0.1262	0.9576
C2	-0.8573	-0.4766	-0.7832	0.1929	1.3382	0.6898
C3	-0.8525	0.9512	-0.2806	-1.1752	1.4607	0.0630
C4	0.3187	1.5594	0.0035	-1.9105	0.3496	-0.1560
C5	1.5760	0.7531	-0.2341	-1.3037	-0.9652	0.2797
C6	1.4184	0.0595	-1.6195	-0.7004	-0.7382	1.6964
C7	1.4113	-0.6673	0.4130	0.1684	-1.0557	-0.2545
C8	0.4376	2.9535	0.5463	-3.2627	0.3501	-0.8053
C9	2.7325	-1.4417	0.4224	0.7719	-2.4489	-0.0554
C10	0.7860	-0.7761	1.7990	0.4482	-0.6232	-1.6900
O11	-1.6109	-1.3502	0.0624	1.2275	1.8791	-0.1672
H12	-2.5105	-0.9953	0.0977	1.0764	2.8268	-0.2478
H13	0.9044	0.6433	-2.3902	-1.2664	-0.0738	2.3576
H14	0.5799	-2.0423	-1.2154	1.5180	-0.2313	1.3996
H15	-1.2878	-0.5038	-1.7993	0.2252	1.8841	1.6459
H16	-1.8095	1.4560	-0.1464	-1.5444	2.4502	-0.2095
H17	-0.5438	3.4261	0.6515	-3.5899	1.3645	-1.0522
H18	0.9264	2.9384	1.5288	-3.2383	-0.2449	-1.7268
H19	1.0574	3.5746	-0.1121	-4.0079	-0.1094	-0.1447
H20	2.3514	-0.3417	-2.0187	-0.4537	-1.6619	2.2214
H21	2.4919	1.3158	-0.0166	-1.9705	-1.8188	0.1095
H22	2.5445	-2.4898	0.6852	1.8539	-2.4004	-0.2221
H23	3.2510	-1.4242	-0.5397	0.6003	-2.8561	0.9444
H24	3.4066	-1.0212	1.1787	0.3426	-3.1475	-0.7839
H25	0.5510	-1.8225	2.0225	1.5281	-0.6134	-1.8696
H26	1.5027	-0.4170	2.5501	-0.0054	-1.3514	-2.3759
H27	-0.1378	-0.2052	1.8889	0.0535	0.3664	-1.9208
O28	-4.2786	-0.1764	0.1873	3.5668	0.2224	-0.2047
H29	-5.0117	-0.5896	-0.2771	2.8677	0.8909	-0.2553
H30	-4.6166	-0.0329	1.0756	4.3262	0.6519	-0.6043