

Supporting Material

Flexibility unleashed in acyclic monoterpenes: conformational space of citronellal revealed by broadband rotational spectroscopy

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1 Broadband spectrum (Neon-seeded expansion)

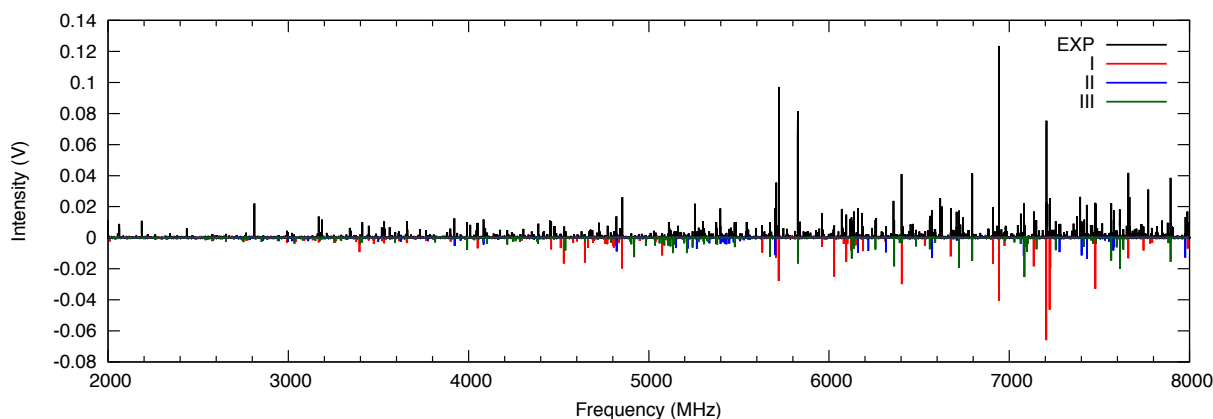


Fig. S1: Full frequency range of the rotational spectrum of citronellal.

2 Dihedral coordinates

The dihedral coordinates reported in Table S1 are defined according to the scheme depicted in Fig. S2.

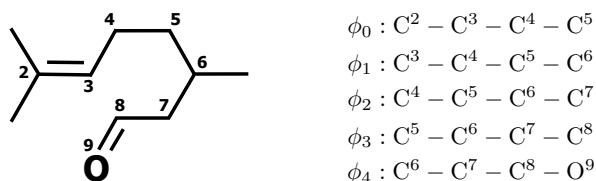


Fig. S2: Schematic view of the chemical structure of citronellal with depicted dihedral coordinates.

Table S1: Dihedral angles for conformations I to XVII of citronellal at the B3LYP-D3/aug-cc-pVTZ level of theory. The conformers are grouped in families according to similar values of ϕ_0 and ϕ_1 . The conformers marked with an asterisk (*) are the ones observed in both Ne and Ar measurements. Conformers marked with (†) are not observed in either due to relaxation.

	ϕ_0	ϕ_1	ϕ_2	ϕ_3	ϕ_4
I*	103.0115	-65.7966	-71.4668	160.8919	-8.1583
IV	111.933	-64.2248	-69.0824	168.2703	125.3858
V†	139.94	-59.5548	-62.5805	78.2307	-135.3349
XVII	125.5718	-57.2352	-52.9374	-54.7099	113.4381
II*	-118.1129	63.0665	-172.1847	165.6228	-5.8736
III*	-122.2383	60.3159	-172.2647	70.8441	5.7601
VI	-118.9618	63.9588	-170.2112	66.0661	-128.5216
X	-120.0746	62.1786	-173.3792	170.261	125.6687
VII*	-90.7836	-179.8446	-165.3682	71.318	5.6918
VIII†	-142.4419	79.918	-57.2651	84.0779	22.9083
IX	110.4994	174.2492	-170.0747	71.52	6.0759
XI*	108.5005	172.4595	-174.4405	165.1503	-5.9939
XII	108.068	179.5411	-69.233	166.0492	-6.9302
XVI*	99.2298	177.9046	56.5703	55.0061	-116.827
XIII*	-109.1934	-174.1171	-67.1224	166.6314	-7.3276
XIV	-111.9047	178.2336	-173.1492	164.7543	-6.0828
XV*	127.2726	-57.1178	-50.3117	-58.2339	-1.1676

3 Predicted barriers for conformer interconversion

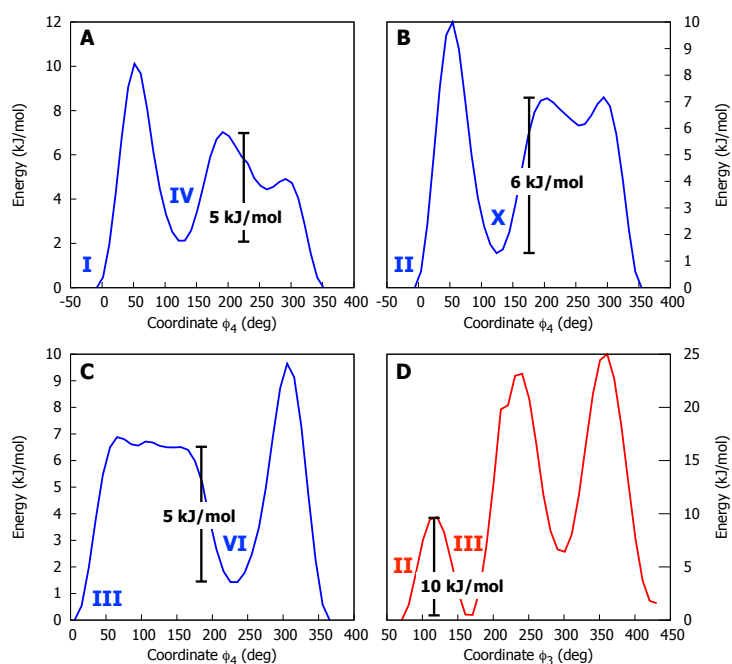


Fig. S3: Energy barriers obtained at the B3LYP-D3/6-311++G** for interconversion between conformers through rotation of single dihedral coordinates as depicted in the figure. Panel A (I - IV); panel B (II - X); panel C (III - VI); panel D (II - III).

4 Predicted energies and spectroscopic parameters

Table S2 shows calculated rotational constants, relative energies and dipole moment components for the lowest seventeen predicted conformations of citronellal at the B3LYP-D3/aug-cc-pVTZ and MP2/6-311+G** levels of theory.

5 Appendix A: line lists

Table S2: Predicted quantum-chemical B3LYP-D3/aug-cc-pVTZ and MP2/6-311++G** structural parameters for the 17 lowest energy conformers of citronellal: relative B3LYP-D3 and MP2 zero-point corrected energies (in cm^{-1}); rotational constants A, B, C (in MHz) and components of the dipole moment μ_a , μ_b , μ_c (in Debye) from the B3LYP-D3 calculation.

	Δ_E (cm^{-1}) B3LYP-D3 ¹	Δ_E (cm^{-1}) MP2 ²	A (MHz)	B (MHz)	C (MHz)	μ_a	μ_b	μ_c
	zero-point	zero-point						
I	0	0	1309	705	564	-0.13	1.37	-1.81
II	111	207	1533	534	481	0.12	-2.20	-0.64
III	137	155	1520	574	502	-0.79	-2.30	-0.55
IV	153	109	1392	584	485	2.91	1.37	-0.03
V	176	192	1366	700	557	-0.92	-2.13	-1.08
VI	211	230	1585	509	458	-2.61	1.78	-1.25
VII	220	417	1605	505	415	-1.35	-1.33	1.22
VIII	224	153	1676	679	600	-0.33	-0.91	1.83
IX	226	451	1893	429	371	-0.22	2.10	-1.66
X	258	242	1779	453	430	-3.10	-0.85	-0.73
XI	259	509	3140	341	327	-1.67	-0.76	1.99
XII	266	563	2549	353	349	-1.70	0.01	1.85
XIII	267	526	2425	377	349	-2.24	-0.87	1.55
XIV	277	559	2641	345	336	-1.39	-0.43	-2.05
XV	356	348	1672	580	526	2.03	0.06	-1.81
XVI	405	437	1525	591	454	1.74	1.82	-0.73
XVII	499	326	1434	638	538	0.04	-2.26	-1.41

Appendix A – Fitted rotational transitions for fifteen conformations of citronellal. Frequencies are shown in MHz.

I

J	Ka	Kc	J'	Ka'	Kc'	Observed	Calculated	Obs-Calc
5	1	5	4	0	4	6095.8886	6095.8759	0.0127
3	2	1	2	1	2	6124.0442	6124.0316	0.0126
3	3	0	2	2	1	7225.8988	7225.8973	0.0015
4	2	2	3	1	2	6943.0172	6943.0322	-0.0150
6	0	6	5	1	5	6910.7733	6910.7843	-0.0110
6	1	6	5	0	5	7136.2206	7136.1947	0.0259
4	2	3	3	1	3	7478.1568	7478.1563	0.0005
5	2	4	4	1	3	7660.5098	7660.5327	-0.0229
4	2	2	3	1	3	7745.1873	7745.1845	0.0028
4	2	3	3	1	2	6675.9767	6676.0040	-0.0273
4	1	3	3	0	3	6402.7128	6402.7030	0.0098
3	3	0	2	2	0	7206.5753	7206.5735	0.0018
3	3	1	2	2	1	7224.1257	7224.1335	-0.0078
3	3	1	2	2	0	7204.8051	7204.8097	-0.0046
5	0	5	4	1	4	5706.8069	5706.8021	0.0048
3	2	1	2	1	1	5722.0694	5722.0736	-0.0042
3	1	2	2	0	2	4853.3025	4853.2866	0.0159
2	2	1	1	1	1	4644.9119	4644.9067	0.0052
5	1	4	4	2	2	4771.1738	4771.1933	-0.0195
2	2	0	1	1	0	4530.2614	4530.2445	0.0169
2	2	1	1	1	0	4510.9170	4510.9207	-0.0037
4	0	4	3	1	3	4458.3526	4458.3476	0.0050
3	1	3	2	0	2	4051.1291	4051.1344	-0.0053
3	2	1	3	1	3	2583.1940	2583.1794	0.0146
3	0	3	2	1	2	3168.1016	3168.0941	0.0075
3	3	1	3	2	2	3470.9746	3470.9819	-0.0073
3	3	0	3	2	2	3472.7413	3472.7458	-0.0045
4	1	3	3	2	1	3446.7655	3446.7655	-0.0000
4	3	1	4	2	3	3532.2103	3532.2140	-0.0037
5	3	3	5	2	4	3612.8740	3612.8809	-0.0069
5	3	2	5	2	4	3660.5179	3660.5078	0.0101
6	2	5	5	3	3	3807.7941	3807.7967	-0.0026
5	0	5	4	1	3	4379.1407	4379.1412	-0.0005
4	4	1	4	3	2	4813.3750	4813.3758	-0.0008
4	4	0	4	3	2	4813.5093	4813.5091	0.0002
4	4	1	4	3	1	4801.1774	4801.1766	0.0008
4	4	0	4	3	1	4801.3087	4801.3099	-0.0012
5	4	2	5	3	3	4806.2625	4806.2612	0.0013
5	4	1	5	3	3	4807.4614	4807.4512	0.0102
6	0	6	5	1	4	4948.6428	4948.6300	0.0128
5	1	4	4	2	3	5038.2106	5038.2215	-0.0109
3	3	1	3	2	1	3376.8634	3376.8874	-0.0240
3	3	0	3	2	1	3378.6334	3378.6513	-0.0179
5	2	4	5	1	5	3136.2491	3136.2541	-0.0050
2	1	2	1	0	1	2993.0610	2993.0646	-0.0036
3	0	3	2	1	1	2766.1226	2766.1361	-0.0135
3	2	2	3	1	3	2489.0827	2489.0848	-0.0021
2	2	1	2	1	2	2276.7850	2276.7856	-0.0006
2	2	0	2	1	2	2296.1166	2296.1094	0.0072
3	2	2	2	1	1	5627.9874	5627.9791	0.0083

Appendix A – Fitted rotational transitions for fifteen conformations of citronellal. Frequencies are shown in MHz.

4 2 3	3 2 2	4989.0711	4989.0715	-0.0004
5 4 2	5 3 2	4758.6429	4758.6343	0.0086
2 2 0	1 1 1	4664.2622	4664.2305	0.0317

II

J	Ka	Kc	J'	Ka'	Kc'	Observed	Calculated	Obs-Calc
3	1	3	2	0	2	3920.9988	3921.0083	-0.0095
5	0	5	4	1	4	4083.1759	4083.1889	-0.0130
4	1	4	3	0	3	4820.9494	4820.9615	-0.0121
5	3	2	5	2	3	5374.1350	5374.1300	0.0050
3	3	0	3	2	1	5408.9034	5408.9102	-0.0068
3	3	1	3	2	2	5417.2249	5417.2272	-0.0023
4	3	2	4	2	3	5421.8237	5421.8179	0.0058
5	3	3	5	2	4	5430.9757	5430.9787	-0.0030
5	1	5	4	0	4	5702.5670	5702.5423	0.0247
3	2	2	2	1	1	6160.6395	6160.6441	-0.0046
3	2	1	2	1	2	6316.5263	6316.5041	0.0222
7	0	7	6	1	6	6218.0184	6218.0249	-0.0065
6	1	6	5	0	5	6570.3510	6570.3383	0.0127
4	2	3	3	1	2	7081.4913	7081.5212	-0.0299
8	0	8	7	1	7	7277.8951	7277.8887	0.0064
4	2	2	3	1	3	7401.4759	7401.4588	0.0171
7	1	7	6	0	6	7429.8066	7429.7849	0.0217
9	4	6	9	3	7	7563.8250	7563.8347	-0.0097
7	4	3	7	3	4	7564.7927	7564.7901	0.0026
7	4	4	7	3	5	7572.1004	7572.1034	-0.0030
6	4	2	6	3	3	7572.4857	7572.4862	-0.0005
6	4	3	6	3	4	7575.4324	7575.4356	-0.0032
5	4	1	5	3	2	7576.9073	7576.8972	0.0101
5	2	4	4	1	3	7977.7622	7977.7796	-0.0174
6	3	3	6	2	4	5335.4518	5335.4472	0.0046
7	3	4	7	2	5	5276.8766	5276.8750	0.0016
2	2	0	1	1	1	5265.7667	5265.7806	-0.0139
8	3	5	8	2	6	5195.5095	5195.5034	0.0061
6	0	6	5	1	5	5151.2893	5151.3038	-0.0145
9	3	6	9	2	7	5090.5579	5090.5659	-0.0080
0	2	8	9	3	7	5067.7876	5067.8047	-0.0171
7	1	6	6	2	5	4363.8133	4363.7792	0.0341
8	2	7	8	1	8	4161.6029	4161.5856	0.0173
7	2	6	7	1	7	3956.1037	3956.1086	-0.0049
6	2	5	6	1	6	3777.2048	3777.2138	-0.0090
5	2	4	5	1	5	3624.7887	3624.8090	-0.0203
6	1	5	5	2	4	3213.7739	3213.7596	0.0143
2	2	0	2	1	1	3177.7055	3177.7046	0.0009
3	2	1	3	1	2	3111.7248	3111.7193	0.0055
4	2	2	4	1	3	3032.1995	3032.1858	0.0137
4	0	4	3	1	3	3019.6896	3019.7012	-0.0116
2	1	2	1	0	1	2999.2485	2999.2551	-0.0066
5	2	3	5	1	4	2946.1955	2946.1805	0.0150
6	2	4	6	1	5	2862.1077	2862.1175	-0.0098

Appendix A – Fitted rotational transitions for fifteen conformations of citronellal. Frequencies are shown in MHz.

7 2 5	7 1 6	2789.1877	2789.2116	-0.0239
5 1 4	4 2 3	2082.1980	2082.2222	-0.0242
4 2 2	3 1 2	7106.4895	7106.4866	0.0029
9 2 8	9 1 9	4393.5118	4393.5050	0.0068
9 2 7	9 1 8	2713.5877	2713.5802	0.0075
8 2 6	8 1 7	2736.7824	2736.7825	-0.0001

III

J	Ka	Kc	J'	Ka'	Kc'	Observed	Calculated	Obs-Calc
1	1	1	0	0	0	2042.3857	2042.3989	-0.0132
3	0	3	2	1	2	2262.4067	2262.4101	-0.0034
6	2	4	6	1	5	2578.7845	2578.8040	-0.0195
5	2	3	5	1	4	2654.8078	2654.8086	-0.0008
2	1	2	1	0	1	3034.1731	3034.1600	0.0131
3	0	3	2	0	2	3174.2070	3174.2091	-0.0021
3	2	2	2	2	1	3189.1894	3189.1920	-0.0026
3	2	2	3	1	3	3261.1387	3261.1333	0.0054
3	1	2	2	1	1	3293.7059	3293.6940	0.0119
4	0	4	3	1	3	3397.7316	3397.7318	-0.0002
4	2	3	4	1	4	3407.9801	3407.9827	-0.0026
5	2	4	5	1	5	3593.0737	3593.0770	-0.0033
3	1	3	2	0	2	3991.7311	3991.7302	0.0009
7	2	6	7	1	7	4079.2981	4079.2871	0.0110
4	1	4	3	1	3	4102.4583	4102.4487	0.0096
4	0	4	3	0	3	4215.2489	4215.2529	-0.0040
4	2	3	3	2	2	4249.3061	4249.2980	0.0081
4	2	2	3	2	1	4286.1989	4286.2060	-0.0071
5	0	5	4	1	4	4538.3382	4538.3463	-0.0081
5	3	2	5	2	3	4983.0010	4982.9929	0.0081
4	3	2	4	2	3	5087.1437	5087.1393	0.0044
5	3	3	5	2	4	5107.1930	5107.2054	-0.0124
5	1	5	4	1	4	5121.7870	5121.7834	0.0036
5	0	5	4	0	4	5243.0625	5243.0632	-0.0007
5	2	4	4	2	3	5306.8886	5306.8777	0.0109
5	3	3	4	3	2	5326.9402	5326.9438	-0.0036
5	3	2	4	3	1	5329.5077	5329.5254	-0.0177
5	2	3	4	2	2	5378.9313	5378.9331	-0.0018
5	1	4	4	1	3	5475.6106	5475.6260	-0.0154
6	0	6	5	1	5	5673.4641	5673.4709	-0.0068
5	1	5	4	0	4	5826.5090	5826.5004	0.0086
6	1	6	5	1	5	6137.5561	6137.5531	0.0030
6	0	6	5	0	5	6256.9107	6256.9080	0.0027
3	2	2	2	1	2	6341.0715	6341.0646	0.0069
3	2	1	2	1	2	6359.7595	6359.7594	0.0001
6	2	5	5	2	4	6361.3331	6361.3203	0.0128
6	3	4	5	3	3	6395.5958	6395.6017	-0.0059
6	3	3	5	3	2	6402.4367	6402.4365	0.0002
6	2	4	5	2	3	6482.3835	6482.3783	0.0052
6	1	5	5	1	4	6558.3754	6558.3828	-0.0074
6	1	6	5	0	5	6720.9825	6720.9903	-0.0078
7	0	7	6	1	6	6794.1401	6794.1418	-0.0017

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7 1 7	6 1 6	7149.6004	7149.6011	-0.0007
7 0 7	6 0 6	7258.2277	7258.2240	0.0037
7 2 6	6 2 5	7412.0630	7412.0440	0.0190
7 3 4	6 3 3	7480.2828	7480.2789	0.0039
4 2 2	3 1 3	7566.0267	7566.0342	-0.0075
7 1 7	6 0 6	7613.6692	7613.6833	-0.0141
7 1 6	6 1 5	7633.2885	7633.2831	0.0054
9 1 8	8 2 7	7881.7776	7881.7863	-0.0087
8 0 8	7 1 7	7894.7927	7894.7837	0.0090

IV

J Ka Kc	J' Ka Kc	Observed	Calculated	Obs-Calc
3 2 1	2 2 0	3237.7198	3237.7273	-0.0075
3 1 2	2 1 1	3348.1396	3348.1390	0.0006
4 1 4	3 1 3	4043.2379	4043.2309	0.0070
4 0 4	3 0 3	4175.6372	4175.6386	-0.0014
4 2 2	3 2 1	4350.1981	4350.2001	-0.0020
3 0 3	2 0 2	3162.3050	3162.3022	0.0028
5 0 5	4 0 4	5162.7918	5162.7916	0.0002
5 2 4	4 2 3	5312.0817	5312.0658	0.0159
5 2 3	4 2 2	5482.3237	5482.3237	-0.0000
5 1 4	4 1 3	5542.6894	5542.6879	0.0015
6 1 6	5 1 5	6028.7422	6028.7418	0.0004
6 0 6	5 0 5	6129.6476	6129.6509	-0.0033
6 2 5	5 2 4	6357.1370	6357.1351	0.0019
6 3 4	5 3 3	6438.2861	6438.2919	-0.0058
6 3 3	5 3 2	6468.2798	6468.2828	-0.0030
6 1 5	5 1 4	6616.2571	6616.2580	-0.0009
6 2 4	5 2 3	6626.3751	6626.3733	0.0018
7 1 7	6 1 6	7011.3299	7011.3256	0.0043
7 0 7	6 0 6	7085.7196	7085.7073	0.0123
7 2 6	6 2 5	7393.2004	7393.2031	-0.0027
7 3 5	6 3 4	7515.2163	7515.2184	-0.0021
7 4 4	6 4 3	7512.9133	7512.9101	0.0032
7 1 6	6 1 5	7666.7379	7666.7351	0.0028
7 2 5	6 2 4	7770.7272	7770.7271	0.0001
8 1 8	7 1 7	7988.3183	7988.3169	0.0014
2 1 2	1 1 1	2030.4134	2030.4102	0.0032
2 0 2	1 0 1	2123.7970	2123.7878	0.0092
2 1 1	1 1 0	2236.2911	2236.2919	-0.0008
4 2 3	3 2 2	4259.2071	4259.2174	-0.0103
8 0 8	7 1 7	7908.2256	7908.2305	-0.0049
4 1 3	3 1 2	4451.6370	4451.6351	0.0019
8 1 7	7 2 6	7460.9339	7460.9335	0.0004
5 2 4	4 1 3	7303.6964	7303.6991	-0.0027
4 2 2	3 1 3	7198.6001	7198.5967	0.0034
7 1 7	6 0 6	7216.3778	7216.3764	0.0014
7 0 7	6 1 6	6880.6486	6880.6565	-0.0079
4 2 3	3 1 2	6443.2703	6443.2684	0.0019
6 1 6	5 0 5	6334.6915	6334.7016	-0.0101

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6 0 6	5 1 5	5823.6977	5823.6910	0.0067
3 2 1	2 1 2	5888.2739	5888.2808	-0.0069
3 2 2	2 1 1	5532.1893	5532.1900	-0.0007
5 1 5	4 0 4	5468.7603	5468.7514	0.0089
6 2 4	6 1 5	2079.6401	2079.6334	0.0067
8 2 6	8 1 7	2399.1570	2399.1590	-0.0020
3 0 3	2 1 2	2478.2884	2478.2842	0.0042
4 1 4	3 0 3	4604.8293	4604.8308	-0.0015
5 0 5	4 1 4	4733.5977	4733.5993	-0.0016
4 2 2	3 0 3	7760.1974	7760.1967	0.0007
5 1 5	4 1 4	5039.5408	5039.5592	-0.0184

VI

J Ka Kc	J' Ka Kc	Observed	Calculated	Obs-Calc
2 1 2	1 0 1	3014.7228	3014.7218	0.0010
4 0 4	3 0 3	3777.7248	3777.7387	-0.0139
4 1 3	3 1 2	3878.9953	3878.9986	-0.0033
3 1 3	2 0 2	3894.7369	3894.7433	-0.0064
3 1 2	2 0 2	4167.5187	4167.5054	0.0133
5 0 5	4 0 4	4712.5518	4712.5477	0.0041
5 2 4	4 2 3	4735.6706	4735.6698	0.0008
4 1 4	3 0 3	4754.2006	4754.1947	0.0059
5 1 4	4 1 3	4846.0287	4846.0308	-0.0021
6 1 6	5 1 5	5539.8175	5539.8141	0.0034
5 1 5	4 0 4	5595.7513	5595.7472	0.0041
6 0 6	5 0 5	5641.3532	5641.3587	-0.0055
6 2 5	5 2 4	5680.2873	5680.2830	0.0043
6 2 4	5 2 3	5724.7461	5724.7458	0.0003
6 1 5	5 1 4	5811.1108	5811.1235	-0.0127
7 1 7	6 1 6	6458.7226	6458.7191	0.0035
7 0 7	6 0 6	6563.6044	6563.6133	-0.0089
7 2 6	6 2 5	6623.5352	6623.5306	0.0046
7 2 5	6 2 4	6693.1691	6693.1649	0.0042
7 1 6	6 1 5	6773.7756	6773.7605	0.0151
8 0 8	7 1 7	6802.5252	6802.5122	0.0130
7 1 7	6 0 6	7240.3712	7240.3740	-0.0028
6 1 5	5 0 5	7375.4951	7375.5027	-0.0076
8 1 8	7 1 7	7375.9053	7375.8923	0.0130
8 0 8	7 0 7	7479.2573	7479.2729	-0.0156
8 2 7	7 2 6	7565.1902	7565.1962	-0.0060
8 3 6	7 3 5	7594.4117	7594.4093	0.0024
8 3 5	7 3 4	7600.2026	7600.2053	-0.0027
8 2 6	7 2 5	7666.4668	7666.4690	-0.0022
8 1 7	7 1 6	7733.3609	7733.3584	0.0025
9 0 9	8 1 8	7815.4902	7815.4960	-0.0058

Appendix A – Fitted rotational transitions for fifteen conformations of citronellal. Frequencies are shown in MHz.

VII

J	Ka	Kc	J'	Ka'	Kc'	Observed	Calculated	Obs-Calc
7	3	5	7	2	5	5269.4006	5269.3826	0.0180
8	3	5	8	2	6	5119.1130	5119.1065	0.0065
5	1	4	4	1	3	4840.1295	4840.1212	0.0083
3	1	3	2	1	2	2643.8861	2643.8961	-0.0100
5	1	5	4	1	4	4390.2639	4390.2709	-0.0070
4	1	4	3	1	3	3519.3040	3519.3165	-0.0125
4	1	3	3	1	2	3881.3697	3881.3790	-0.0093
4	2	3	3	2	2	3706.9888	3706.9925	-0.0037
3	1	2	2	1	1	2916.1392	2916.1607	-0.0215
6	1	6	5	1	5	5256.2917	5256.3032	-0.0115
6	0	6	5	0	5	5395.3383	5395.3571	-0.0188
6	2	4	5	2	3	5713.4870	5713.5067	-0.0197
7	1	7	6	1	6	6117.2921	6117.3037	-0.0116
7	0	7	6	0	6	6239.1478	6239.1544	-0.0066
7	2	6	6	2	5	6452.5679	6452.5689	-0.0010
7	2	5	6	2	4	6707.0306	6707.0489	-0.0183
7	1	6	6	1	5	6728.2073	6728.2148	-0.0075
5	2	4	4	2	3	4626.9418	4626.9424	-0.0006
5	2	3	4	2	2	4729.7658	4729.7760	-0.0102
8	0	8	7	0	7	7072.7090	7072.7075	0.0015
8	2	7	7	2	6	7356.7097	7356.7009	0.0088
8	3	6	7	3	5	7464.1704	7464.1403	0.0301
8	1	7	7	1	6	7651.5943	7651.5941	0.0002
8	2	6	7	2	5	7703.9774	7703.9984	-0.0210
9	1	9	8	1	8	7825.2828	7825.2906	-0.0078
9	0	9	8	0	8	7901.3365	7901.3392	-0.0027
4	1	3	3	0	3	5318.8168	5318.8164	0.0004
2	2	0	1	1	1	5330.9942	5330.9880	0.0062
3	1	3	2	0	2	3654.5840	3654.5842	-0.0002
5	0	5	4	1	4	3782.2263	3782.2438	-0.0175
4	2	3	4	1	4	3887.9965	3887.9828	0.0137
4	1	4	3	0	3	4412.0091	4412.0118	-0.0027
5	0	5	4	0	4	4536.0875	4536.0684	0.0191
5	1	5	4	0	4	5144.0929	5144.0955	-0.0026
7	3	5	6	3	4	6527.6482	6527.6262	0.0220
7	3	4	6	3	3	6552.2976	6552.2923	0.0053
5	3	3	5	2	3	5571.1585	5571.1778	-0.0193
5	3	2	5	2	3	5576.8052	5576.8020	0.0032
6	3	3	5	3	2	5602.2733	5602.2655	0.0078
4	3	2	4	2	3	5725.3240	5725.3392	-0.0152
5	3	3	5	2	4	5753.9412	5753.9525	-0.0113
5	3	2	5	2	4	5759.5566	5759.5767	-0.0201
7	0	7	6	1	6	5770.1750	5770.1812	-0.0062
6	3	4	6	2	5	5802.6760	5802.6804	-0.0044
6	3	3	6	2	5	5819.4280	5819.4358	-0.0078
6	1	6	5	0	5	5864.3320	5864.3303	0.0017
7	3	5	7	2	6	5877.7328	5877.7377	-0.0049
7	3	4	7	2	6	5919.1371	5919.1593	-0.0222
8	3	6	8	2	7	5985.1706	5985.1771	-0.0065
3	2	2	2	1	1	6071.7365	6071.7253	0.0112

Appendix A – Fitted rotational transitions for fifteen conformations of citronellal. Frequencies are shown in MHz.

3 2 1	2 1 1	6098.6877	6098.6652	0.0225
9 3 7	9 2 8	6130.5072	6130.5156	-0.0084
3 2 2	2 1 2	6344.2052	6344.2028	0.0024
3 2 1	2 1 2	6371.1491	6371.1428	0.0063
5 1 4	4 0 4	6500.7666	6500.7504	0.0162
7 1 7	6 0 6	6586.2739	6586.2769	-0.0030
8 0 8	7 1 7	6725.5816	6725.5850	-0.0034
4 2 3	3 1 2	6862.5675	6862.5571	0.0104
4 2 2	3 1 2	6942.5114	6942.4982	0.0132
4 2 2	3 1 3	7487.2480	7487.2404	0.0076
5 2 4	4 1 3	7608.1235	7608.1205	0.0030
9 0 9	8 1 8	7653.4383	7653.4441	-0.0058
6 1 5	5 0 5	7754.7104	7754.6879	0.0225
5 2 3	4 1 3	7790.9002	7790.8953	0.0049
1 1 1	0 0 0	2023.8991	2023.9108	-0.0117
4 0 4	3 1 3	2765.4759	2765.4920	-0.0161
3 0 3	2 0 2	2761.8994	2761.8890	0.0104
2 1 2	1 0 1	2860.8916	2860.8940	-0.0024
8 2 6	8 1 7	2905.4930	2905.5133	-0.0203
5 2 3	5 1 4	2950.7810	2950.7741	0.0069
2 1 1	1 0 1	3133.3679	3133.3715	-0.0036
6 0 6	5 1 5	4787.3195	4787.3301	-0.0106
6 2 5	5 2 4	5542.4190	5542.4064	0.0126
6 1 5	6 0 6	2359.3279	2359.3308	-0.0029
5 2 4	5 1 5	4124.6644	4124.6543	0.0101
4 3 1	4 2 3	5726.7675	5726.7509	0.0166
8 3 5	7 3 4	7512.3297	7512.3008	0.0289

IX

J Ka Kc	J' Ka Kc	Observed	Calculated	Obs-Calc
8 1 8	7 0 7	7046.8967	7046.8906	0.0061
6 1 6	5 0 5	5766.4404	5766.4433	-0.0029
7 1 7	6 0 6	6409.8062	6409.8123	-0.0061
4 1 4	3 0 3	4436.9763	4436.9751	0.0012
9 1 9	8 0 8	7683.7687	7683.7601	0.0086
3 2 1	2 1 2	6985.6777	6985.6777	-0.0000
3 2 2	2 1 1	6805.6535	6805.6565	-0.0030
2 2 1	1 1 0	6055.5466	6055.5503	-0.0037
3 2 2	3 1 3	4642.2559	4642.2653	-0.0094
7 0 7	6 1 6	4584.5431	4584.5630	-0.0199
3 2 1	3 1 2	4306.9650	4306.9766	-0.0116
4 2 2	4 1 3	4210.9876	4210.9955	-0.0079
3 1 3	2 0 2	3740.7385	3740.7625	-0.0240
8 0 8	7 1 7	5483.7187	5483.7147	0.0040
2 2 0	1 1 1	6114.4607	6114.4604	0.0003
5 1 5	4 0 4	5110.6807	5110.6784	0.0023
8 3 6	8 2 7	7540.4239	7540.4325	-0.0086
4 2 2	3 1 3	7895.0875	7895.0830	0.0045
5 0 5	4 1 4	2780.2047	2780.2027	0.0020
4 2 3	3 1 3	7870.4301	7870.4234	0.0067

Appendix A – Fitted rotational transitions for fifteen conformations of citronellal. Frequencies are shown in MHz.

9 3 6	9 2 8	7618.1705	7618.1705	0.0000
9 3 7	9 2 8	7591.1034	7591.0952	0.0082
8 3 5	8 2 7	7554.0429	7554.0438	-0.0009
4 2 2	3 1 2	7551.5551	7551.5529	0.0022
7 3 4	7 2 6	7510.2766	7510.2740	0.0026
7 3 5	7 2 6	7504.0621	7504.0636	-0.0015
6 3 3	6 2 5	7481.7989	7481.7983	0.0006
5 3 2	5 2 4	7464.4195	7464.4231	-0.0036
5 3 3	5 2 4	7463.5926	7463.5917	0.0009
4 3 2	4 2 3	7454.5176	7454.5318	-0.0142
4 3 1	4 2 3	7454.7455	7454.7399	0.0056
5 3 3	5 2 3	7406.3459	7406.3414	0.0045
5 3 2	5 2 3	7407.1817	7407.1728	0.0089
6 3 3	6 2 4	7368.2760	7368.2688	0.0072
6 3 4	6 2 4	7365.7700	7365.7784	-0.0084
7 3 5	7 2 5	7302.3567	7302.3676	-0.0109
7 3 4	7 2 5	7308.5856	7308.5780	0.0076
10 0 10	9 1 9	7249.2474	7249.2549	-0.0075
8 3 6	8 2 6	7210.4884	7210.4767	0.0117
9 3 6	9 2 7	7112.4074	7112.4055	0.0019
3 2 2	2 1 2	6977.4365	6977.4364	0.0001
10 3 7	10 2 8	6973.4827	6973.4942	-0.0115
6 1 5	5 0 5	6966.4289	6966.4121	0.0168
12 3 9	12 2 10	6627.9139	6627.9156	-0.0017
9 0 9	8 1 8	6373.2968	6373.3009	-0.0041
2 2 0	1 1 0	6057.1978	6057.2004	-0.0026
5 1 4	4 0 4	5968.7562	5968.7464	0.0098
8 2 7	8 1 8	5527.7445	5527.7451	-0.0006
7 2 6	7 1 7	5289.3672	5289.3715	-0.0043
5 1 5	4 0 4	5110.6802	5110.6784	0.0018
6 2 5	6 1 6	5081.9013	5081.9080	-0.0067
4 1 3	3 0 3	5009.3634	5009.3667	-0.0033
5 2 3	5 1 5	4962.3883	4962.3907	-0.0024
5 2 4	5 1 5	4905.1423	4905.1404	0.0019
4 2 2	4 1 4	4783.3786	4783.3871	-0.0085
4 2 3	4 1 4	4758.7355	4758.7275	0.0080
3 2 1	3 1 3	4650.5020	4650.5066	-0.0046
2 2 1	2 1 2	4555.3577	4555.3486	0.0091
2 2 0	2 1 2	4557.0104	4556.9987	0.0117
3 1 2	2 0 2	4084.2856	4084.2926	-0.0070
3 2 1	2 1 1	6813.8937	6813.8978	-0.0041
6 0 6	5 1 5	3681.3146	3681.2982	0.0164
2 1 2	1 0 1	3018.6388	3018.6608	-0.0220
5 2 3	5 1 4	4104.3560	4104.3227	0.0333

X

J Ka Kc	J' Ka Kc	Observed	Calculated	Obs-Calc
9 1 9	8 1 8	7742.6086	7742.6035	0.0051
9 0 9	8 0 8	7819.3857	7819.3931	-0.0074
9 2 8	8 2 7	7846.9085	7846.8850	0.0235

Appendix A – Fitted rotational transitions for fifteen conformations of citronellal. Frequencies are shown in MHz.

9 2 7	8 2 6	7879.3238	7879.3489	-0.0251
9 1 8	8 1 7	7945.1250	7945.1149	0.0101
8 1 8	7 1 7	6883.7695	6883.7727	-0.0032
8 0 8	7 0 7	6956.5499	6956.5599	-0.0100
8 1 7	7 1 6	7064.0917	7064.1176	-0.0259
8 2 7	7 2 6	6976.1338	6976.1055	0.0283
7 1 7	6 1 6	6024.4504	6024.4553	-0.0049
7 1 6	6 1 5	6182.4464	6182.4569	-0.0105
7 0 7	6 0 6	6091.7075	6091.7141	-0.0066
6 1 6	5 1 5	5164.6829	5164.6948	-0.0119
6 1 5	5 1 4	5300.2356	5300.2349	0.0007
5 1 5	4 1 4	4304.5353	4304.5413	-0.0060
5 1 4	4 1 3	4417.5519	4417.5458	0.0061
5 0 5	4 0 4	4356.7231	4356.7274	-0.0043
5 2 4	4 2 3	4361.6646	4361.6402	0.0244
5 2 3	4 2 2	4367.1847	4367.1685	0.0162
4 1 4	3 1 3	3444.0458	3444.0511	-0.0053
4 0 4	3 0 3	3487.0483	3487.0505	-0.0022
4 1 3	3 1 2	3534.4820	3534.4775	0.0045
3 1 2	2 1 1	2651.1126	2651.1123	0.0003
3 0 3	2 0 2	2616.2603	2616.2640	-0.0037
7 2 5	6 2 4	6120.3197	6120.3178	0.0019
8 2 6	7 2 5	6999.0457	6999.0312	0.0145
6 2 4	5 2 3	5243.0625	5243.0856	-0.0231
6 2 5	5 2 4	5233.4521	5233.4352	0.0169

XI

J Ka Kc	J' Ka Kc	Observed	Calculated	Obs-Calc
6 1 6	5 1 5	4009.0523	4009.0612	-0.0089
5 1 4	4 1 3	3410.8691	3410.8736	-0.0045
6 0 6	5 0 5	4049.5426	4049.5475	-0.0049
6 2 4	5 2 3	4053.0197	4053.0227	-0.0030
7 1 6	6 1 5	4774.8131	4774.8180	-0.0049
7 0 7	6 0 6	4723.6542	4723.6585	-0.0043
4 1 3	3 1 2	2728.7797	2728.7850	-0.0053
8 1 7	7 1 6	5456.6451	5456.6431	0.0020
8 0 8	7 0 7	5397.3907	5397.3955	-0.0048
9 1 9	8 1 8	6012.6601	6012.6531	0.0070
9 0 9	8 0 8	6070.7014	6070.7068	-0.0054
9 2 8	8 2 7	6076.1086	6076.1051	0.0035
9 2 7	8 2 6	6082.4108	6082.4094	0.0014
8 2 7	7 2 6	5401.2057	5401.2059	-0.0002
3 1 3	2 1 2	2004.7237	2004.7213	0.0024
3 1 2	2 1 1	2046.6556	2046.6389	0.0167
8 2 6	7 2 5	5405.6211	5405.6227	-0.0016
7 2 6	6 2 5	4726.2260	4726.2277	-0.0017
4 1 4	3 1 3	2672.8960	2672.8955	0.0005
5 1 4	4 0 4	6262.0368	6262.0431	-0.0063
6 1 6	6 0 6	2636.8529	2636.8567	-0.0038
7 1 7	7 0 7	2590.2319	2590.2239	0.0080

Appendix A – Fitted rotational transitions for fifteen conformations of citronellal. Frequencies are shown in MHz.

8 1 8	8 0 8	2537.7161	2537.7222	-0.0061
6 1 5	5 1 4	4092.8879	4092.8896	-0.0017
7 2 5	6 2 4	4729.1725	4729.1740	-0.0015
1 1 0	0 0 0	3462.8621	3462.8694	-0.0073
4 1 3	3 0 3	5551.5798	5551.5840	-0.0042
2 1 1	1 0 1	4152.1028	4152.0812	0.0216
3 1 3	2 0 2	4764.4725	4764.4626	0.0099
4 1 4	3 0 3	5411.8535	5411.8593	-0.0058
5 1 5	4 0 4	6052.4523	6052.4582	-0.0059
6 1 6	5 0 5	6686.3915	6686.4043	-0.0128
7 1 7	6 0 6	7313.8915	7313.8824	0.0091
2 1 2	2 0 2	2759.7260	2759.7413	-0.0153
11 0 11	10 0 10	7415.8441	7415.8525	-0.0084
11 2 10	10 2 9	7425.6355	7425.6277	0.0078
11 1 11	10 1 10	7347.7897	7347.7975	-0.0078
11 2 9	10 2 8	7437.1590	7437.1529	0.0061
4 0 4	3 0 3	2700.4315	2700.4144	0.0171
3 1 2	2 0 2	4848.3244	4848.2979	0.0265
5 1 5	4 1 4	3341.0071	3341.0134	-0.0063
10 0 10	9 1 8	3635.2304	3635.2228	0.0076
7 1 7	6 1 6	4677.0316	4677.0257	0.0059

XII

J Ka Kc	J' Ka Kc	Observed	Calculated	Obs-Calc
9 1 9	8 1 8	6359.0877	6359.0862	0.0015
9 0 9	8 0 8	6376.8556	6376.8454	0.0102
8 1 8	7 1 7	5652.5798	5652.5694	0.0104
8 0 8	7 0 7	5668.4607	5668.4503	0.0104
7 1 7	6 1 6	4946.0457	4946.0356	0.0101
7 1 6	6 1 5	4974.4602	4974.4510	0.0092
6 1 6	5 1 5	4239.4785	4239.4869	-0.0084
6 0 6	5 0 5	4251.5112	4251.5147	-0.0035
5 1 5	4 1 4	3532.9159	3532.9253	-0.0094
5 0 5	4 0 4	3542.9839	3542.9869	-0.0030
4 1 4	3 1 3	2826.3506	2826.3531	-0.0025
4 0 4	3 0 3	2834.4177	2834.4274	-0.0097
4 1 3	3 1 2	2842.5912	2842.5908	0.0004
10 1 10	9 1 9	7065.5814	7065.5840	-0.0026
10 0 10	9 0 9	7085.1950	7085.1838	0.0112
11 1 11	10 1 10	7772.0512	7772.0607	-0.0095
11 0 11	10 0 10	7793.4560	7793.4591	-0.0031
11 1 10	10 1 9	7816.6993	7816.7084	-0.0091
6 1 5	5 1 4	4263.8512	4263.8432	0.0080
8 2 6	7 2 5	5669.3110	5669.3174	-0.0064
8 2 7	7 2 6	5668.8385	5668.8498	-0.0113
9 1 8	8 1 7	6395.6056	6395.6189	-0.0133
10 1 9	9 1 8	7106.1783	7106.1746	0.0037
11 2 10	10 2 9	7794.4897	7794.4926	-0.0029
5 1 4	4 1 3	3553.2220	3553.2224	-0.0004
11 2 9	10 2 8	7795.7292	7795.7167	0.0125

Appendix A – Fitted rotational transitions for fifteen conformations of citronellal. Frequencies are shown in MHz.

XIII

J	Ka	Kc	J'	Ka'	Kc'	Observed	Calculated	Obs-Calc
3	1	3	2	1	2	2156.9893	2156.9984	-0.0091
3	1	2	2	1	1	2239.0905	2239.1017	-0.0112
6	1	5	6	0	6	2358.9808	2358.9635	0.0173
1	1	0	0	0	0	2803.1254	2803.1120	0.0134
4	0	4	3	0	3	2928.1975	2928.2246	-0.0271
4	1	3	3	1	2	2985.1329	2985.1396	-0.0067
2	1	2	1	0	1	3481.1337	3481.1160	0.0177
2	1	1	1	0	1	3563.2319	3563.2211	0.0108
5	1	5	4	1	4	3594.0829	3594.0841	-0.0012
5	0	5	4	0	4	3658.2073	3658.2277	-0.0204
5	2	4	4	2	3	3663.0694	3663.0752	-0.0058
5	3	3	4	3	2	3664.5979	3664.6033	-0.0054
5	2	3	4	2	2	3668.5188	3668.5296	-0.0108
5	1	4	4	1	3	3730.8688	3730.8901	-0.0213
3	1	3	2	0	2	4172.9236	4172.9047	0.0189
6	1	6	5	1	5	4312.1527	4312.1601	-0.0074
3	1	2	2	0	2	4337.1223	4337.1130	0.0093
6	0	6	5	0	5	4386.8774	4386.8732	0.0042
6	2	5	5	2	4	4395.1802	4395.1738	0.0064
6	2	4	5	2	3	4404.6926	4404.7032	-0.0106
6	1	5	5	1	4	4476.2782	4476.2748	0.0034
4	1	4	3	0	3	4851.4713	4851.4527	0.0186
7	1	7	6	1	6	5029.8192	5029.8471	-0.0279
7	0	7	6	0	6	5113.8865	5113.9081	-0.0216
4	1	3	3	0	3	5125.1384	5125.1242	0.0142
7	2	6	6	2	5	5126.9943	5126.9909	0.0034
7	2	5	6	2	4	5142.1944	5142.1967	-0.0023
7	1	6	6	1	5	5221.2142	5221.2110	0.0032
5	1	5	4	0	4	5517.3304	5517.3122	0.0182
8	1	8	7	1	7	5747.0692	5747.0928	-0.0236
8	0	8	7	0	7	5839.0728	5839.0991	-0.0263
8	2	7	7	2	6	5858.4855	5858.4798	0.0057
8	2	6	7	2	5	5881.1988	5881.1948	0.0040
5	1	4	4	0	4	5927.7849	5927.7896	-0.0047
8	1	7	7	1	6	5965.6239	5965.6108	0.0131
5	2	4	5	1	4	5965.8943	5965.9110	-0.0167
5	2	3	5	1	5	6385.9275	6385.9379	-0.0104
6	2	5	6	1	6	6459.3853	6459.4021	-0.0168
9	1	9	8	1	8	6463.8257	6463.8503	-0.0246
6	2	4	6	1	6	6478.4706	6478.4810	-0.0104
9	0	9	8	0	8	6562.2492	6562.2422	0.0070
9	2	8	8	2	7	6589.5952	6589.5940	0.0012
7	2	5	7	1	7	6590.8210	6590.8306	-0.0096
9	2	7	8	2	6	6621.8562	6621.8524	0.0038
9	1	8	8	1	7	6709.3973	6709.3800	0.0173
6	1	5	5	0	5	6745.8571	6745.8366	0.0205
7	1	7	6	0	6	6814.2457	6814.2185	0.0272
10	0	10	9	0	9	7283.1823	7283.1742	0.0081
10	2	9	9	2	8	7320.2994	7320.2872	0.0122
10	2	8	9	2	7	7364.2942	7364.2832	0.0110

Appendix A – Fitted rotational transitions for fifteen conformations of citronellal. Frequencies are shown in MHz.

8 1 8	7 0 7	7447.4144	7447.4032	0.0112
10 1 9	9 1 8	7452.4433	7452.4174	0.0259
11 1 11	10 1 10	7895.7095	7895.7435	-0.0340
4 1 4	3 1 3	2875.6966	2875.6765	0.0201

XIV

J Ka Kc	J' Ka Kc	Observed	Calculated	Obs-Calc
6 0 6	5 0 5	4139.2818	4139.2832	-0.0014
5 0 5	4 0 4	3449.7279	3449.7300	-0.0021
6 1 6	5 1 5	4109.7218	4109.7015	0.0203
5 1 4	4 1 3	3475.7117	3475.7080	0.0037
6 1 5	5 1 4	4170.7387	4170.7331	0.0056
7 1 7	6 1 6	4794.4958	4794.5039	-0.0081
7 1 6	6 1 5	4865.6902	4865.6941	-0.0039
7 0 7	6 0 6	4828.6186	4828.6228	-0.0042
8 1 8	7 1 7	5479.2326	5479.2393	-0.0067
8 0 8	7 0 7	5517.7151	5517.7138	0.0013
8 2 6	7 2 5	5523.0954	5523.0902	0.0052
8 2 7	7 2 6	5520.2344	5520.2329	0.0015
8 1 7	7 1 6	5560.5724	5560.5797	-0.0073
9 1 9	8 1 8	6163.8968	6163.8986	-0.0018
9 0 9	8 0 8	6206.5109	6206.5217	-0.0108
9 1 8	8 1 7	6255.3848	6255.3786	0.0062
10 1 10	9 1 9	6848.4732	6848.4734	-0.0002
11 1 11	10 1 10	7532.9582	7532.9555	0.0027
11 0 11	10 0 10	7583.1640	7583.1548	0.0092
11 2 10	10 2 9	7589.5474	7589.5533	-0.0059

XV

J Ka Kc	J' Ka Kc	Observed	Calculated	Obs-Calc
3 1 3	2 1 2	3217.6248	3217.6260	-0.0012
3 0 3	2 0 2	3291.6744	3291.6776	-0.0032
5 1 5	4 1 4	5356.6979	5356.6951	0.0028
5 0 5	4 0 4	5461.2773	5461.2844	-0.0071
5 2 4	4 2 3	5494.5540	5494.5536	0.0004
5 1 4	4 1 3	5624.1412	5624.1607	-0.0195
6 0 6	5 0 5	6534.1399	6534.1469	-0.0070
6 1 6	5 1 5	6423.3811	6423.3719	0.0092
6 2 4	5 2 3	6654.2903	6654.2791	0.0112
6 1 5	5 1 4	6743.0375	6743.0299	0.0076
7 1 7	6 1 6	7487.8581	7487.8575	0.0006
7 0 7	6 0 6	7598.3163	7598.3193	-0.0030
7 2 6	6 2 5	7683.3902	7683.3929	-0.0027
7 1 6	6 1 5	7858.2471	7858.2504	-0.0033
4 1 4	3 1 3	4288.0224	4288.0195	0.0029
4 1 3	3 1 2	4502.4477	4502.4502	-0.0025
3 1 2	2 0 2	4590.8095	4590.8044	0.0051

Appendix A – Fitted rotational transitions for fifteen conformations of citronellal. Frequencies are shown in MHz.

5 2 3	4 2 2	5532.0570	5532.0638	-0.0068
5 1 4	4 0 4	7045.6434	7045.6470	-0.0036
7 2 5	6 2 4	7783.2125	7783.2066	0.0059
3 1 2	2 1 1	3378.6169	3378.5980	0.0189

XVI

J Ka Kc	J' Ka Kc	Observed	Calculated	Obs-Calc
3 1 2	2 1 1	3323.1774	3323.1807	-0.0033
3 1 3	2 0 2	3711.7308	3711.7336	-0.0028
4 1 4	3 1 3	3866.9388	3866.9509	-0.0121
4 0 4	3 0 3	4033.9527	4033.9249	0.0278
4 2 3	3 2 2	4157.0633	4157.0458	0.0175
4 2 2	3 2 1	4291.2457	4291.2574	-0.0117
5 0 5	4 1 4	4487.2404	4487.2508	-0.0104
4 1 4	3 0 3	4508.5975	4508.5998	-0.0023
5 0 5	4 0 4	4961.9422	4961.9256	0.0166
5 2 4	4 2 3	5178.5401	5178.5395	0.0006
5 1 5	4 0 4	5287.3352	5287.3346	0.0006
5 2 3	4 2 2	5426.4573	5426.4410	0.0163
5 1 4	4 1 3	5481.7932	5481.7850	0.0082
6 0 6	5 1 5	5539.4271	5539.4340	-0.0069
6 1 6	5 1 5	5748.4020	5748.3917	0.0103
7 1 6	6 2 5	5852.2380	5852.2294	0.0086
6 0 6	5 0 5	5864.8229	5864.8429	-0.0200
3 2 2	2 1 1	5897.9603	5897.9395	0.0208
6 1 6	5 0 5	6073.7979	6073.8007	-0.0028
6 2 5	5 2 4	6188.5264	6188.5350	-0.0086
6 3 4	5 3 3	6307.3182	6307.3084	0.0098
6 3 3	5 3 2	6356.7956	6356.7894	0.0062
3 2 1	2 1 2	6381.2037	6381.1911	0.0126
6 1 5	5 1 4	6524.7562	6524.7493	0.0069
7 0 7	6 1 6	6547.7802	6547.7857	-0.0055
6 2 4	5 2 3	6574.1813	6574.1704	0.0109
7 1 7	6 1 6	6675.2176	6675.2169	0.0007
4 2 3	3 1 2	6731.7912	6731.8046	-0.0134
7 0 7	6 0 6	6756.7338	6756.7434	-0.0096
7 1 7	6 0 6	6884.1724	6884.1747	-0.0023
5 4 1	5 3 2	6892.4437	6892.4339	0.0098
7 2 6	6 2 5	7185.3200	7185.3376	-0.0176
7 3 5	6 3 4	7362.5894	7362.5860	0.0034
7 3 4	6 3 3	7468.5855	7468.5901	-0.0046
5 2 4	4 1 3	7498.3442	7498.3560	-0.0118
7 1 6	6 1 5	7532.5828	7532.5861	-0.0033
8 1 8	7 1 7	7594.8026	7594.7932	0.0094
8 0 8	7 0 7	7647.4934	7647.4789	0.0145
7 2 5	6 2 4	7717.0025	7717.0193	-0.0168
8 1 8	7 0 7	7722.2259	7722.2244	0.0015
4 2 2	3 1 3	7761.2428	7761.2696	-0.0268

Appendix A – Fitted rotational transitions for fifteen conformations of citronellal. Frequencies are shown in MHz.

XVII

J	Ka	Kc	J'	Ka'	Kc'	Observed	Calculated	Obs-Calc
2	1	2	1	0	1	3036.0182	3036.0196	-0.0014
5	1	4	4	2	3	3979.2514	3979.2557	-0.0043
4	0	4	3	1	3	3999.1174	3999.1137	0.0037
5	3	2	5	2	3	4053.3787	4053.3825	-0.0038
3	1	3	2	0	2	4056.6300	4056.6339	-0.0039
2	2	1	1	1	0	4838.5500	4838.5569	-0.0069
4	1	4	3	0	3	5042.0984	5042.0978	0.0006
5	0	5	4	1	4	5224.4873	5224.4898	-0.0025
3	2	2	2	1	1	5905.9227	5905.9217	0.0010
5	1	5	4	0	4	6009.4947	6009.4941	0.0006
3	2	2	2	1	2	6207.8270	6207.8242	0.0028
3	2	1	2	1	2	6251.8930	6251.8824	0.0106
6	0	6	5	1	5	6422.4044	6422.3984	0.0060
4	2	3	3	1	2	6921.8548	6921.8528	0.0020
6	1	6	5	0	5	6977.1943	6977.1940	0.0003
4	2	3	3	1	3	7525.1631	7525.1595	0.0036
7	0	7	6	1	6	7588.0670	7588.0619	0.0051
4	2	2	3	1	3	7654.3004	7654.3132	-0.0128
3	3	0	2	2	1	7764.6129	7764.6085	0.0044
5	2	4	4	1	3	7888.1527	7888.1560	-0.0033
7	1	7	6	0	6	7959.1198	7959.1258	-0.0060