Supplementary data

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Assigned rotational transitions of eucalyptol

J'	K_a'	K_c'	J	K_a	K_c	obs (MHz)	o-c (kHz)
9	3	6	9	2	7	2057.719	-2.3
7	2	6	7	1	7	2064.004	1.7
13	2	11	13	1	12	2119.183	-1.1
8	3	5	8	2	6	2152.844	-0.9
10	1	9	10	0	10	2163.796	7.6
7	3	4	7	2	5	2241.108	3.3
6	3	3	6	2	4	2313.989	-2.5
5	3	2	5	2	3	2367.275	-2.5
4	3	1	4	2	2	2401.213	1.0
3	3	0	3	2	1	2419.439	2.8
14	2	12	14	1	13	2430.518	-5.1
3	3	1	3	2	2	2432.545	-1.2
9	2	8	9	1	9	2435.195	2.4
18	4	14	18	3	15	2437.311	-5.4
4	3	2	4	2	3	2439.629	2.9
19	4	15	19	3	16	2449.572	1.5
5	3	3	5	2	4	2453.594	-3.2
6	3	4	6	2	5	2477.337	4.9
17	4	13	17	3	14	2478.014	6.4

J'	K_a'	K_c'	J	K_a	K_c	obs (MHz)	o-c (kHz)
11	1	10	11	0	11	2498.399	-2.5
7	3	5	7	2	6	2513.781	-0.7
20	4	16	20	3	17	2521.994	0.2
16	4	12	16	3	13	2561.551	-6.6
8	3	6	8	2	7	2565.774	-1.7
9	3	7	9	2	8	2635.842	6.0
10	2	9	10	1	10	2649.879	-0.7
21	4	17	21	3	18	2658.883	11.7
15	4	11	15	3	12	2675.346	-1.5
10	3	8	10	2	9	2726.021	-2.8
15	2	13	15	1	14	2771.219	0.8
14	4	10	14	3	11	2805.217	-1.9
12	1	11	12	0	12	2836.505	0.0
11	3	9	11	2	10	2837.817	-2.3
22	4	18	22	3	19	2861.244	1.0
11	2	10	11	1	11	2881.285	0.8
13	4	9	13	3	10	2937.133	0.3
19	3	16	19	2	17	2959.425	2.3
12	3	10	12	2	11	2972.042	0.8
23	5	18	23	4	19	3027.462	4.4
25	5	20	25	4	21	3043.068	-4.8
12	4	8	12	3	9	3059.083	2.4
22	5	17	22	4	18	3107.496	-6.0
12	2	11	12	1	12	3127.046	-2.4
13	3	11	13	2	12	3128.803	-1.1
16	2	14	16	1	15	3129.469	-2.3
11	4	7	11	3	8	3162.707	-0.7
13	1	12	13	0	13	3171.589	-0.2
21	5	16	21	4	17	3231.019	6.3
10	4	6	10	3	7	3244.117	3.1
9	4	5	9	3	6	3303.524	7.9
14	3	12	14	2	13	3307.527	2.5
8	4	4	8	3	5	3343.975	12.4
7	4	3	7	3	4	3369.744	2.2
7	4	3	7	3	4	3369.744	2.2

J'	K_a'	K_c'	J	K_a	K_c	obs (MHz)	o-c (kHz)
20	5	15	20	4	16	3383.413	-6.9
13	2	12	13	1	13	3384.738	3.1
6	4	2	6	3	3	3385.124	3.0
8	4	5	8	3	6	3389.186	-3.8
8	4	5	8	3	6	3389.194	4.2
7	4	4	7	3	5	3390.928	-1.9
5	4	1	5	3	2	3393.667	5.4
6	4	3	6	3	4	3393.776	-5.8
10	4	7	10	3	8	3396.551	2.1
5	4	2	5	3	3	3396.592	-1.0
4	4	0	4	3	1	3398.019	4.6
4	4	1	4	3	2	3398.752	-3.0
11	4	8	11	3	9	3410.657	0.0
12	4	9	12	3	10	3435.608	0.9
12	4	9	12	3	10	3435.610	3.3
24	4	20	24	3	21	3447.101	2.7
13	4	10	13	3	11	3474.440	6.9
17	2	15	17	1	16	3494.169	0.2
14	1	13	14	0	14	3500.136	-4.8
15	3	13	15	2	14	3506.976	4.2
19	5	14	19	4	15	3549.102	0.6
15	4	12	15	3	13	3604.827	-1.0
14	2	13	14	1	14	3651.985	-0.1
16	4	13	16	3	14	3700.888	6.2
18	5	13	18	4	14	3713.292	0.0
16	3	14	16	2	15	3725.369	-3.2
17	4	14	17	3	15	3819.493	-1.0
15	1	14	15	0	15	3821.114	-2.8
18	2	16	18	1	17	3856.566	4.0
17	5	12	17	4	13	3864.012	-0.2
15	2	14	15	1	15	3926.643	-6.4
17	3	15	17	2	16	3960.551	-1.8
18	4	15	18	3	16	3961.266	-5.1
16	5	11	16	4	12	3993.449	4.3
15	5	10	15	4	11	4098.314	-4.5

J'	K'_a	K'_c	J	K_a	K_c	obs (MHz)	o-c (kHz)
19	4	16	19	3	17	4126.080	2.4
14	5	9	14	4	10	4179.212	-2.0
16	2	15	16	1	16	4206.869	1.3
18	3	16	18	2	17	4210.110	0.4
18	3	16	18	2	17	4210.112	2.8
13	5	8	13	4	9	4239.181	0.5
12	5	7	12	4	8	4282.294	2.5
15	5	11	15	4	12	4299.755	-7.3
16	5	12	16	4	13	4302.709	-13.1
14	5	10	14	4	11	4303.749	-12.2
13	5	9	13	4	10	4312.073	-3.5
11	5	6	11	4	7	4312.583	-4.4
12	5	8	12	4	9	4322.496	-9.5
11	5	7	11	4	8	4333.356	-1.0
10	5	5	10	4	6	4333.514	-5.9
18	5	14	18	4	15	4341.440	-8.2
10	5	6	10	4	7	4343.458	-3.9
9	5	4	9	4	5	4347.782	-0.2
9	5	5	9	4	6	4352.125	-3.9
8	5	3	8	4	4	4357.363	3.0
8	5	4	8	4	5	4359.055	-2.7
7	5	2	7	4	3	4363.673	4.5
7	5	3	7	4	4	4364.231	-10.1
6	5	1	6	4	2	4367.716	12.8
6	5	2	6	4	3	4367.858	-2.6
5	5	0	5	4	1	4370.176	8.6
5	5	1	5	4	2	4370.196	-3.2
19	5	15	19	4	16	4383.302	-3.7
19	5	15	19	4	16	4383.308	2.1
17	1	16	17	0	17	4443.015	3.6
20	5	16	20	4	17	4443.898	-2.9
20	2	18	20	1	19	4555.407	-9.6
20	3	18	20	2	19	4742.594	6.3
18	1	17	18	0	18	4746.427	3.6
21	6	15	21	5	16	4813.268	1.2

J'	K'_a	K'_c	J	K_a	K_c	obs (MHz)	o-c (kHz)
21	2	19	21	1	20	4889.282	-1.0
24	5	20	24	4	21	4909.811	1.9
20	6	14	20	5	15	4937.663	8.3
19	2	18	19	1	19	5067.109	-2.1
18	6	12	18	5	13	5113.146	5.4
21	6	16	21	5	17	5166.713	2.7
22	6	17	22	5	18	5167.688	5.7
17	6	11	17	5	12	5171.556	1.8
23	6	18	23	5	19	5180.961	-0.8
19	6	14	19	5	15	5189.526	8.0
18	6	13	18	5	14	5207.826	1.1
16	6	10	16	5	11	5215.721	-3.3
17	6	12	17	5	13	5227.746	0.2
16	6	11	16	5	12	5247.628	-5.6
15	6	9	15	5	10	5249.035	-6.2
15	6	10	15	5	11	5266.315	-6.4
14	6	8	14	5	9	5274.192	-1.7
14	6	9	14	5	10	5283.076	0.8
13	6	7	13	5	8	5293.223	7.2
13	6	8	13	5	9	5297.522	2.5
12	6	6	12	5	7	5307.606	1.6
12	6	7	12	5	8	5309.547	-6.2
11	6	5	11	5	6	5318.455	3.3
11	6	6	11	5	7	5319.261	-5.5
10	6	4	10	5	5	5326.566	6.3
10	6	5	10	5	6	5326.858	-11.0
9	6	3	9	5	4	5332.549	19.5
9	6	4	9	5	5	5332.617	-16.6
8	6	3	8	5	4	5336.841	-14.8
7	6	1	7	5	2	5339.823	2.8
7	6	2	7	5	3	5339.823	-4.1
6	6	0	6	5	1	5341.818	0.5
6	6	1	6	5	2	5341.818	-0.6
21	2	20	21	1	21	5648.216	0.6
25	7	18	25	6	19	5766.891	9.8

J'	K_a'	K_c'	J	K_a	K_c	obs (MHz)	o-c (kHz)
23	7	16	23	6	17	5971.578	3.3
22	7	15	22	6	16	6043.286	5.8
23	7	17	23	6	18	6082.714	-14.5
21	7	14	21	6	15	6099.850	1.7
22	7	16	22	6	17	6112.078	3.5
21	7	15	21	6	16	6141.019	1.8
20	7	13	20	6	14	6144.623	-0.2
20	7	14	20	6	15	6168.414	0.0
19	7	12	19	6	13	6180.276	1.0
19	7	13	19	6	14	6193.521	-3.2
18	7	11	18	6	12	6208.854	5.3
18	7	12	18	6	13	6215.942	2.1
17	7	10	17	6	11	6231.880	4.7
17	7	11	17	6	12	6235.510	0.8
16	7	9	16	6	10	6250.485	-5.7
16	7	10	16	6	11	6252.262	-3.6
15	7	8	15	6	9	6265.547	4.5
15	7	9	15	6	10	6266.356	-7.7
14	7	7	14	6	8	6277.685	12.3
14	7	8	14	6	9	6278.025	-4.6
13	7	6	13	6	7	6287.399	17.3
13	7	7	13	6	8	6287.509	-17.4
11	7	4	11	6	5	6301.087	12.1
11	7	5	11	6	6	6301.087	-6.0
10	7	3	10	6	4	6305.681	4.8
10	7	4	10	6	5	6305.681	-0.5
9	7	2	9	6	3	6309.124	2.3
9	7	3	9	6	4	6309.124	0.9
8	7	1	8	6	2	6311.630	2.0
8	7	2	8	6	3	6311.630	1.8
7	7	0	7	6	1	6313.388	2.5
7	7	1	7	6	2	6313.388	2.4
22	8	14	22	7	15	7138.832	0.1
22	8	15	22	7	16	7144.127	-19.5
21	8	13	21	7	14	7165.302	1.9

J'	K_a'	K_c'	J	K_a	K_c	obs (MHz)	o-c (kHz)
21	8	14	21	7	15	7168.126	4.6
20	8	12	20	7	13	7187.610	-4.3
19	8	11	19	7	12	7206.445	4.6
19	8	12	19	7	13	7207.143	-5.8
18	8	10	18	7	11	7222.309	12.0
18	8	11	18	7	12	7222.619	-10.7
16	8	8	16	7	9	7246.698	-1.8
16	8	8	16	7	9	7246.711	11.4
16	8	9	16	7	10	7246.760	-2.2
15	8	7	15	7	8	7255.896	12.5
15	8	8	15	7	9	7255.896	-12.2
14	8	6	14	7	7	7263.410	1.2
14	8	7	14	7	8	7263.410	-7.8
13	8	5	13	7	6	7269.505	3.4
13	8	6	13	7	7	7269.505	0.4
12	8	4	12	7	5	7274.364	-0.3
12	8	5	12	7	6	7274.364	-1.2
11	8	3	11	7	4	7278.179	-0.8
11	8	4	11	7	5	7278.179	-1.0
10	8	2	10	7	3	7281.116	2.5
10	8	3	10	7	4	7281.116	2.5
9	8	1	9	7	2	7283.317	2.6
9	8	2	9	7	3	7283.317	2.6
1	1	1	0	0	0	2584.822	1.0
2	0	2	1	1	1	3770.722	-1.8
2	1	2	1	0	1	4662.688	1.3
3	1	3	2	2	0	4770.766	-0.3
3	1	2	2	2	1	5022.523	-2.6
2	2	1	1	1	0	5676.595	-0.7
2	2	0	1	1	1	5720.788	-0.1
3	0	3	2	1	2	5921.099	-0.1
4	2	3	3	3	0	6042.877	0.8
4	2	2	3	3	1	6082.135	-6.0
3	1	3	2	0	2	6720.832	1.3
4	1	4	3	2	1	6791.523	-2.7

J'	K_a'	K_c'	J	K_a	K_c	obs (MHz)	o-c (kHz)
5	3	3	4	4	0	7206.311	8.8
5	3	2	4	4	1	7209.264	-4.9
4	1	3	3	2	2	7219.343	-1.8
3	2	2	2	1	1	7754.461	0.6
3	2	1	2	1	2	7892.285	3.7
4	0	4	3	1	3	8078.470	5.1
5	2	4	4	3	1	8150.716	-3.1
4	1	4	3	0	3	8762.710	2.2
3	3	1	2	2	0	8788.085	-4.3
3	3	0	2	2	1	8790.858	4.4

Table 1: Assigned rotational transitions eucalyptol

Table 2: Assigned rotational transitions for eucalytol with ^{13}C substituted at the C1 position

J'	K_a'	K_c'	J	K_a	K_c	obs (MHz)	o-c (kHz)
2	2	0	1	1	1	5715.493	14
2	2	1	1	1	0	5671.236	4.6
3	0	3	2	1	2	5898.138	-6.7
3	1	3	2	0	2	6703.041	-3.1
3	2	2	2	1	1	7742.259	4.3
4	0	4	3	1	3	8048.877	-5.1
7	6	1	7	5	2	5370.003	-3.5
7	6	2	7	5	3	5370.003	-10.4

Table 3: Assigned rotational transitions for eucalytol with ^{13}C substituted at the C2/C6 position

J'	K_a'	K_c'	J	K_a	K_c	obs (MHz)	o-c (kHz)
2	1	2	1	0	1	4642.668	8.3
2	2	0	1	1	1	5688.029	1.1
2	2	1	1	1	0	5647.475	2
3	0	3	2	1	2	5888.084	3.7
3	1	3	2	0	2	6694.533	-0.9
3	2	1	2	1	2	7843.765	10
3	2	2	2	1	1	7717.593	-4
3	3	0	2	2	1	8743.039	22.8
3	3	1	2	2	0	8740.652	-7.8
4	0	4	3	1	3	8033.027	-12.1
4	1	3	3	2	2	7168.983	-0.1
5	4	2	5	3	3	3377.026	-2.3
7	6	1	7	5	2	5308.883	9.1
7	6	2	7	5	3	5308.883	4.4
9	7	2	9	6	3	6272.777	0.3
9	7	3	9	6	4	6272.777	-0.5
10	7	3	10	6	4	6269.838	3.8
10	7	4	10	6	5	6269.838	0.4
11	5	7	11	4	8	4312.204	-15.4
12	4	8	12	3	9	3090.723	1.5

Table 4: Assigned rotational transitions for eucalytol with ^{13}C substituted at the C3/C5 position

J'	K_a'	K_c'	J	K_a	K_c	obs (MHz)	o-c (kHz)
2	1	2	1	0	1	4630.995	5.3
2	2	0	1	1	1	5666.763	14.1
2	2	1	1	1	0	5620.495	-0.1
3	0	3	2	1	2	5911.296	-4.8
3	1	3	2	0	2	6678.64	5.2
3	2	1	2	1	2	7833.215	2.6
3	2	2	2	1	1	7688.604	-7.4
4	0	4	3	1	3	8060.567	-6.3
5	4	1	5	3	2	3300.881	6.2
6	3	4	6	2	5	2417.005	1.3
6	4	3	6	3	4	3301.439	4.7
6	6	0	6	5	1	5197.227	-4.9
6	6	1	6	5	2	5197.227	-6.5
7	4	3	7	3	4	3273.491	2.1
7	4	4	7	3	5	3298.669	8.6
8	5	4	8	4	5	4239.515	-23.1
9	8	1	9	7	2	7086.045	4.2
9	8	2	9	7	3	7086.045	4.2

Table 5: Assigned rotational transitions for eucalytol with ^{13}C substituted at the C4 position

J'	K'_a	K'_c	J	K_a	K_c	obs (MHz)	o-c (kHz)
2	2	0	1	1	1	5702.2055	4.0
2	2	0	1	1	1	5702.2055	4.0
16	7	9	16	6	10	6200.9458	2.4
8	7	1	8	6	2	6271.4509	3.0
8	7	2	8	6	3	6271.4509	2.6
3	1	3	2	0	2	6692.6641	-1.8
4	0	4	3	1	3	8061.6982	-0.6
9	7	2	9	6	3	6268.5733	-5.1
9	7	3	9	6	4	6268.5733	-7.2

Table 6: Assigned rotational transitions for eucalytol with ^{13}C substituted at the C7 position

J'	K'_a	K'_c	J	K_a	K_c	obs (MHz)	o-c (kHz)
2	1	2	1	0	1	4606.759	-8.3
2	2	1	1	1	0	5633.812	17.6
3	0	3	2	1	2	5834.305	-4.4
4	0	4	3	1	3	7964.755	-1.4
4	4	0	4	1	3	7156.013	54.9
5	4	2	5	3	3	3430.955	41.3
6	4	3	6	3	4	3427.923	36.5
9	4	6	9	3	7	3426.023	32.7

Table 7: Assigned rotational transitions for eucalytol with ^{13}C substituted at the C8 position

J'	K'_a	K'_c	J	K_a	K_c	obs (MHz)	o-c (kHz)
2	2	0	1	1	1	5715.946	4.4
2	2	1	1	1	0	5671.758	-2.8
3	0	3	2	1	2	5898.422	13.2
3	1	3	2	0	2	6703.691	1.3
3	2	2	2	1	1	7742.972	-1.1
4	0	4	3	1	3	8049.249	-10.8

Table 8: Assigned rotational transitions for eucalytol with ^{13}C substituted at the C9/C10 position

J'	K'_a	K'_c	J	K_a	K_c	obs (MHz)	o-c (kHz)
2	0	2	1	1	1	3722.87	-0.0007
2	1	2	1	0	1	4623.617	0
2	2	0	1	1	1	5679.221	0.0138
2	2	1	1	1	0	5638.195	-0.0006
3	0	3	2	1	2	5849.303	-0.0021
3	1	3	2	0	2	6663.317	-0.0084
3	2	1	2	1	2	7823.935	-0.0068
3	2	2	2	1	1	7696.364	0.0073
4	0	4	3	1	3	7983.109	0.0013
6	6	0	6	5	1	5361.858	-0.0109
6	6	1	6	5	2	5361.858	-0.0117
7	4	3	7	3	4	3387.116	-0.0026
7	7	0	7	6	1	6337.056	0.0194
7	7	1	7	6	2	6337.056	0.0194
8	7	1	8	6	2	6335.513	-0.0029
8	7	2	8	6	3	6335.513	-0.0031
9	7	2	9	6	3	6333.338	-0.0098
9	7	3	9	6	4	6333.338	-0.0107
12	5	7	12	4	8	4313.069	0.0032

J'	K'_a	K'_c	J	K_a	K_c	obs (MHz)	o-c (kHz)
1	1	1	0	0	0	2814.091	-3.43
1	1	0	0	0	0	2877.738	0.54
9	2	7	9	1	8	3072.061	3.91
8	2	6	8	1	7	3073.268	-2.96
7	2	5	7	1	6	3118.445	-9.45
2	1	2	1	1	1	3178.179	13.09
5	2	4	5	1	4	3208.49	3.92
2	0	2	1	0	1	3239.331	0.57
3	2	2	3	1	2	3485.682	-0.64
3	2	1	3	1	2	3498.05	-0.72
3	0	3	2	1	1	3529.863	-7.14
2	2	1	2	1	1	3579.581	14.12
2	2	0	2	1	1	3582.036	-9.69
3	0	3	2	1	2	3720.808	7.37
3	2	1	3	1	3	3879.848	-2.01
4	2	3	4	1	4	3997.616	-4.77
4	2	2	4	1	4	4034.55	-0.1
5	2	4	5	1	5	4161.45	0.62
2	1	2	1	0	1	4371.357	0.87
2	1	1	1	0	1	4562.288	1.78
3	1	3	2	1	2	4765.738	8.05
3	0	3	2	0	2	4852.829	3.27
4	0	4	3	1	2	5032.347	17.23
4	0	4	3	1	3	5414.129	-0.85
3	1	3	2	0	2	5897.751	-4.15
5	3	2	5	2	3	6062.975	-2.71
4	3	2	4	2	2	6096.334	-10.5
4	3	1	4	2	2	6096.769	2.45
3	3	1	3	2	1	6114.178	-17.68
3	3	0	3	2	1	6114.266	9.73
3	3	1	3	2	2	6126.553	-11.16
3	3	0	3	2	2	6126.634	9.95
4	3	2	4	2	3	6133.276	2.68
4	3	1	4	2	3	6133.703	7.13
5	3	3	5	2	4	6146.699	15.46
5	3	2	5	2	4	6148.366	-3.74
6	3	4	6	2	5	6169.823	0.67
7	3	5	7	2	6	6206.019	-0.76
3	1	2	2	0	2	6279.562	7.17
4	1	4	3	1	3	6351.549	-4.75
4	0	4	3	0	3	6459.057	-2.07
4	2	3	3	2	2	6481.686	-7.1
6	1	5	5	2	4	6686.334	8.85
2	2	1	1	1	0	6885.016	-3.95
2	2	0	1	1	0	6887.495	-2.75
2	2	1	1	1	1	6948.663	0.52
2	2	0	1	1	1	6951.143	2.02
5	0	5	4	1	4	7118.611	-20.47
4	1	4	3	0	3	7396.492	8.73
3	2	1	2	1	2	8645.578	-1.75
2	2	1	2	1	2	3770.512	14.83
2	1	1	1	1	0	3305.454	1.23
3	2	2	2	2	1	4862.696	-19.3

Table 9: Assigned rotational transitions of 1,4-cineole