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Structure determination of *trans*-cinnamaldehyde by broadband microwave spectroscopy - Supplementary Material

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Contents

1 Rotational Constants of the ^{13}C isotopologues

Table 1: Experimentally determined rotational constants for all nine single ^{13}C substituted species of *s-trans-trans*-cinnamaldehyde, number of assigned lines and the error of the fit are given in this table. The distortion constants D_J, D_K and D_{JK} of the parent molecule were used for the fits of the isotopologues.

Isotopologue	A (MHz)	B (MHz)	C (MHz)	assigned lines	error (kHz)
C1	4863.49(83)	571.91382(56)	512.04405(57)	17	7.6
C2	4866.23(81)	576.58248(68)	515.80562(79)	12	7.9
C3	4848.36(59)	578.55109(52)	517.21422(54)	15	6.9
C4	4863.91(32)	578.89400(19)	517.65356(19)	13	2.5
C5	4791.14(67)	577.61341(69)	515.80867(68)	14	8.3
C6	4823.39(69)	573.75216(60)	513.07512(60)	22	8.7
C7	4860.67(70)	572.07195(61)	512.16369(63)	18	8.0
C8	4780.37(85)	575.50095(36)	513.98454(32)	13	4.5
C9	4813.79(61)	578.44614(43)	516.70858(48)	15	6.3

2 Coordinates from the substitution method

Table 2: Experimentally determined atom positions, calculated with the substitution method, are given in this table.

Atom number	x	y
C(1)	3.30890(14)	-0.31446(235)
C(2)	1.94040(28)	0.23460(401)
C(3)	0.87748(47)	-0.60873(111)
C(4)	-0.50070(39)	-0.23877(127)
C(5)	-1.47934(36)	-1.27512(67)
C(6)	-2.84562(17)	-0.97925(79)
C(7)	-3.27169(15)	0.33589(240)
C(8)	-2.32516(13)	1.37839(33)
C(9)	-0.96338(36)	1.08289(55)

The z-coordinate of the molecule is assumed to be zero in the Kraitchman equations for planar molecules.

3 Details of the $r_m^{(1)}$-fit

Adjustable constant from the $r_m^{(1)}$-fit:

$c_c = -0.0218 \pm 0.0013$

Coordinates from the substitution method:

Table 3: Experimentally determined atom positions, calculated with the substitution method, are given in this table.

Atom number	x	y
C(1)	3.3172(88)	-0.310(12)
C(2)	1.94040(28)	0.23460(401)
C(3)	0.87748(47)	-0.60873(111)
C(4)	-0.50070(39)	-0.23877(127)
C(5)	-1.47934(36)	-1.27512(67)
C(6)	-2.84562(17)	-0.97925(79)
C(7)	-3.27169(15)	0.33589(240)
C(8)	-2.32516(13)	1.37839(33)
C(9)	-0.96338(36)	1.08289(55)

4 Comparison between the Bond Lengths of the *s-trans*- and the *s-cis*-Conformers in *trans*-cinnamaldehyde and acrolein

***trans*-cinnamaldehyde**

Table 4: Comparison of the calculated bond length of *s-cis-trans*- and *s-trans-trans*-cinnamaldehyde from *ab initio* calculations using the MP2/6-311++(2d,2p) functional.

bond lengths [Å]	*s-trans-trans*-cinnamaldehyde	*s-cis-trans*-cinnamaldehyde
C1-C2	1.465	1.477
C2-C3	1.350	1.348
C3-C4	1.460	1.460
C4-C5	1.403	1.404
C5-C6	1.394	1.394
C6-C7	1.395	1.395
C7-C8	1.398	1.398
C8-C9	1.391	1.391
C9-C4	1.405	1.404

Table 5: Comparison of the calculated bond angles of *s-cis-trans-* and *s-trans-trans*-cinnamaldehyde from *ab initio* calculations using the MP2/6-311++(2d,2p) functional.

bond angles [°]	*s-trans-trans*-cinnamaldehyde	*s-cis-trans*-cinnamaldehyde
C1-C2-C3	119.67	120.76
C2-C3-C4	127.32	127.13
C3-C4-C5	118.73	118.50
C4-C5-C6	120.89	120.92
C5-C6-C7	119.94	119.98
C6-C7-C8	119.69	119.66
C7-C8-C9	120.38	120.38
C8-C9-C4	120.46	120.53
C9-C4-C5	118.63	118.54

acrolein(ref)

Table 6: Comparison of the experimentally determined bond length of *s-cis-* and *s-trans*-acrolein (ref).

bond lengths [Å]	*s-trans*-acrolein	*s-cis*-acrolein
C1-C2	1.468(4)	1.478(6)
C2-C3	1.340(4)	1.340(7)

Table 7: Comparison of the experimentally determined bond angle of *s-cis-* and *s-trans*-acrolein (ref).

bond angle [°]	*s-trans*-acrolein	*s-cis*-acrolein
C1-C2-C3	119.7(3)	121.5(6)

5 Line List of Observed Transitions

In the following table the assigned transitions for the two conformers of trans-cinnamaldehyde and the single substituted species are listed. The quantum numbers describe a transition from $J'_{K'_a K'_c} \leftarrow J_{K_a K_c}$. The observed and the calculated frequency and their difference for each transition are given in the table.

Conformer 1: *s-trans-trans*-cinnamaldehyde

J'	K'_a	K'_c	J	K_a	K_c	ν_{obs}[MHz]	ν_{calc}[MHz]	ν_{obs}-ν_{calc} [kHz]
2	1	2	1	1	1	2132.507	2132.508	-0.9
2	0	2	1	0	1	2193.100	2193.100	0.8
8	1	7	8	1	8	2202.737	2202.737	-0.5
2	1	1	1	1	0	2254.997	2254.994	2.8
12	1	11	11	2	10	2497.701	2497.692	8.2
11	2	9	12	1	12	2712.634	2712.638	-3.6
9	1	8	9	1	9	2751.921	2751.921	-0.7
3	1	3	2	1	2	3198.354	3198.356	-2.1
10	2	8	11	1	11	3285.110	3285.115	-5.0
3	0	3	2	0	2	3288.021	3288.021	0.0
3	2	2	2	2	1	3290.621	3290.624	-3.4
3	2	1	2	2	0	3293.223	3293.229	-6.3
3	1	2	2	1	1	3382.081	3382.081	0.0
16	3	13	17	2	16	3664.481	3664.484	-3.1
9	2	7	10	1	10	3924.773	3924.779	-6.5
7	0	7	6	1	6	3931.092	3931.087	4.8
13	1	12	12	2	11	3957.033	3957.028	5.1
11	1	10	11	1	11	4029.041	4029.044	-3.6
14	3	12	15	2	13	4068.961	4068.964	-2.8
4	1	4	3	1	3	4263.721	4263.724	-3.3
1	1	0	1	0	1	4348.560	4348.561	-1.2
4	0	4	3	0	3	4380.997	4380.990	6.3
4	2	3	3	2	2	4386.999	4386.991	8.2
4	2	2	3	2	1	4393.501	4393.501	-0.1
2	1	1	2	0	2	4410.452	4410.455	-3.3
6	2	5	7	1	6	4432.172	4432.171	0.7
3	1	2	3	0	3	4504.519	4504.515	3.7
4	1	3	3	1	2	4508.665	4508.669	-4.1
8	2	6	9	1	9	4626.014	4626.001	13.2
4	1	3	4	0	4	4632.195	4632.194	0.2
12	1	11	12	1	12	4755.345	4755.346	-0.7
5	1	4	5	0	5	4795.421	4795.411	9.7
6	1	5	6	0	6	4996.519	4996.524	-4.6
8	0	8	7	1	7	5196.473	5196.475	-1.6
7	1	6	7	0	7	5238.293	5238.287	5.5
5	1	5	4	1	4	5328.457	5328.461	-3.9
7	2	5	8	1	8	5383.312	5383.310	2.3
1	1	1	0	0	0	5384.196	5384.194	1.9
13	3	11	14	2	12	5399.901	5399.899	1.7
14	1	13	13	2	12	5437.501	5437.504	-2.8
5	0	5	4	0	4	5471.371	5471.367	3.8
5	2	4	4	2	3	5482.921	5482.923	-1.8
5	4	1	4	4	0	5485.809	5485.809	0.5
5	4	2	4	4	1	5485.809	5485.809	0.7

J'	K'_a	K'_c	J	K_a	K_c	ν_{obs}[MHz]	ν_{calc}[MHz]	ν_{obs}-ν_{calc} [kHz]
5	2	3	4	2	2	5495.939	5495.929	10.3
8	1	7	8	0	8	5523.781	5523.787	-5.8
8	1	7	8	0	8	5523.781	5523.787	-5.6
13	1	12	13	1	13	5538.636	5538.628	7.4
5	1	4	4	1	3	5634.579	5634.584	-4.6
9	1	8	9	0	9	5856.344	5856.345	-0.9
6	2	4	7	1	7	6191.558	6191.550	8.1
10	1	9	10	0	10	6239.381	6239.396	-14.8
6	1	6	5	1	5	6392.413	6392.426	-12.9
2	1	2	1	0	1	6419.833	6419.826	6.5
9	0	9	8	1	8	6474.001	6474.010	-8.6
13	3	10	14	2	13	6554.830	6554.819	11.4
6	0	6	5	0	5	6558.518	6558.526	-8.8
6	2	5	5	2	4	6578.316	6578.311	4.8
6	4	2	5	4	1	6583.440	6583.446	-5.8
6	4	3	5	4	2	6583.440	6583.445	-4.9
6	3	4	5	3	3	6584.694	6584.700	-5.8
6	3	3	5	3	2	6584.941	6584.942	-1.0
6	2	4	5	2	3	6601.021	6601.029	-7.7
11	1	10	11	0	11	6676.329	6676.324	5.0
12	3	10	13	2	11	6693.563	6693.558	4.7
6	1	5	5	1	4	6759.641	6759.639	1.9
15	1	14	14	2	13	6937.221	6937.233	-12.0
4	2	3	5	1	4	7014.216	7014.215	1.1
5	2	3	6	1	6	7045.994	7046.007	-12.9
12	1	11	12	0	12	7170.276	7170.281	-5.1
3	1	3	2	0	2	7425.079	7425.083	-3.2
7	1	7	6	1	6	7455.480	7455.486	-6.0
7	0	7	6	0	6	7641.862	7641.876	-14.2
7	2	6	6	2	5	7673.051	7673.047	4.2
7	5	2	6	5	1	7680.403	7680.401	2.3
7	5	3	6	5	2	7680.403	7680.401	2.3
7	4	4	6	4	3	7681.340	7681.341	-0.2
7	4	3	6	4	2	7681.340	7681.344	-3.1
7	3	5	6	3	4	7683.262	7683.252	9.8
7	3	4	6	3	3	7683.793	7683.797	-4.3
7	2	5	6	2	4	7709.285	7709.284	0.8
13	1	12	13	0	13	7723.993	7723.982	11.3
10	0	10	9	1	9	7759.666	7759.654	11.8
7	1	6	6	1	5	7883.632	7883.639	-7.0
4	2	2	5	1	5	7942.508	7942.503	5.2
11	3	9	12	2	10	7952.526	7952.538	-12.7
8	1	8	7	1	7	8517.535	8517.524	11.1
8	0	8	7	0	7	8720.887	8720.874	13.4
8	2	7	7	2	6	8767.029	8767.022	6.5
8	3	5	7	3	4	8783.339	8783.343	-4.4
8	2	6	7	2	5	8821.119	8821.125	-5.6
8	1	7	7	1	6	9006.372	9006.374	-1.2
9	1	9	8	1	8	9578.450	9578.434	16.0

Table 8: Observed Transitions of the *s-trans-trans*-conformer

Conformer 2: *s-cis-trans*-cinnamaldehyde

J'	K'_a	K'_c	J	K_a	K_c	ν_{obs}[MHz]	ν_{calc}[MHz]	ν_{obs}-ν_{calc} [kHz]
5	0	5	4	1	4	2318.438	2318.439	-1.0
3	1	3	2	1	2	3413.266	3413.270	-3.7
3	0	3	2	0	2	3523.621	3523.621	-0.7
3	1	2	2	1	1	3641.467	3641.468	-1.2
1	1	0	1	0	1	3944.133	3944.131	1.6
2	1	1	2	0	2	4021.317	4021.311	5.5
3	1	2	3	0	3	4139.138	4139.158	-20.3
5	1	4	5	0	5	4507.493	4507.492	1.2
4	1	4	3	1	3	4549.746	4549.753	-7.0
4	0	4	3	0	3	4692.999	4692.989	10.4
4	2	3	3	2	2	4703.212	4703.221	-8.7
4	2	2	3	2	1	4714.321	4714.312	9.4
4	1	3	3	1	2	4853.967	4853.970	-2.2
7	0	7	6	1	6	5002.141	5002.143	-1.8
7	1	6	7	0	7	5077.615	5077.612	3.6
8	1	7	8	0	8	5449.770	5449.765	4.5
5	1	5	4	1	4	5685.181	5685.175	6.3
5	0	5	4	0	4	5857.954	5857.955	-1.8
9	1	8	9	0	9	5886.605	5886.606	-1.0
5	2	3	4	2	2	5899.764	5899.776	-11.3
5	1	4	4	1	3	6065.300	6065.308	-8.1
2	1	2	1	0	1	6144.041	6144.035	6.2
8	0	8	7	1	7	6366.961	6366.960	1.1
10	1	9	10	0	10	6392.908	6392.910	-2.3
6	1	6	5	1	5	6819.307	6819.307	0.0
6	0	6	5	0	5	7017.505	7017.497	7.7
6	2	5	5	2	4	7051.133	7051.129	4.0
6	2	4	5	2	3	7089.738	7089.734	3.9
3	1	3	2	0	2	7206.371	7206.373	-1.8
6	1	5	5	1	4	7275.162	7275.154	7.7
9	0	9	8	1	8	7739.227	7739.228	-0.9
9	3	6	10	2	9	7907.519	7907.519	0.0
7	1	7	6	1	6	7951.937	7951.944	-7.1
7	0	7	6	0	6	8170.688	8170.688	-0.2
7	2	6	6	2	5	8223.512	8223.511	0.6

Table 9: Observed Transitions of the *s-cis-trans*-conformer

Isotopologue C1

J'	K'_a	K'_c	J	K_a	K_c	ν_{obs}[MHz]	ν_{calc}[MHz]	ν_{obs}-ν_{calc} [kHz]
3	0	3	2	0	2	3249.370	3249.385	-15.1
3	1	2	2	1	1	3341.295	3341.286	8.9
4	1	4	3	1	3	4214.855	4214.857	-2.0
4	0	4	3	0	3	4329.610	4329.613	-2.3
4	2	3	3	2	2	4335.330	4335.343	-12.9
4	1	3	3	1	2	4454.301	4454.312	-10.6
5	1	5	4	1	4	5267.431	5267.430	0.9
5	0	5	4	0	4	5407.353	5407.364	-10.5
5	2	3	4	2	2	5430.826	5430.820	6.4
5	1	4	4	1	3	5566.691	5566.694	-3.1

J'	K'_a	K'_c	J	K_a	K_c	ν_{obs}[MHz]	ν_{calc}[MHz]	ν_{obs}-ν_{calc} [kHz]
6	1	6	5	1	5	6319.272	6319.264	8.1
6	0	6	5	0	5	6482.036	6482.041	-4.4
6	2	4	5	2	3	6522.632	6522.633	-0.4
6	1	5	5	1	4	6678.261	6678.257	4.7
7	1	7	6	1	6	7370.235	7370.233	1.5
7	0	7	6	0	6	7553.082	7553.075	6.3
7	1	6	6	1	5	7788.822	7788.813	8.4

Table 10: Observed Transitions of the C1-^{13}C-substituted species

Isotopologue C2

J'	K'_a	K'_c	J	K_a	K_c	ν_{obs}[MHz]	ν_{calc}[MHz]	ν_{obs}-ν_{calc} [kHz]
3	0	3	2	0	2	3274.601	3274.599	2.1
4	0	4	3	0	3	4363.140	4363.142	-1.7
4	1	3	3	1	2	4489.800	4489.808	-7.7
5	1	5	4	1	4	5307.244	5307.231	13.3
5	0	5	4	0	4	5449.121	5449.132	-10.7
5	1	4	4	1	3	5611.019	5611.027	-7.9
6	1	6	5	1	5	6366.961	6366.976	-14.4
6	0	6	5	0	5	6531.961	6531.954	6.9
6	1	5	5	1	4	6731.401	6731.400	1.2
7	0	7	6	0	6	7611.028	7611.025	3.4
7	2	5	6	2	4	7677.392	7677.387	4.1
7	1	6	6	1	5	7850.742	7850.735	6.2

Table 11: Observed Transitions of the C2-^{13}C-substituted species

Isotopologue C3

J'	K'_a	K'_c	J	K_a	K_c	ν_{obs}[MHz]	ν_{calc}[MHz]	ν_{obs}-ν_{calc} [kHz]
3	0	3	2	0	2	3284.661	3284.671	-10.2
4	1	3	3	1	2	4504.401	4504.406	-5.4
5	1	5	4	1	4	5322.661	5322.654	7.3
5	0	5	4	0	4	5465.721	5465.722	-1.0
5	3	3	4	3	2	5481.021	5481.024	-3.2
5	1	4	4	1	3	5629.251	5629.246	4.8
6	1	6	5	1	5	6385.438	6385.445	-6.6
6	0	6	5	0	5	6551.694	6551.702	-8.1
6	2	4	5	2	3	6594.515	6594.507	7.3
6	1	5	5	1	4	6753.221	6753.220	0.6
7	1	7	6	1	6	7447.336	7447.325	10.6
7	0	7	6	0	6	7633.842	7633.846	-3.6
7	2	6	6	2	5	7665.239	7665.237	1.6
7	2	5	6	2	4	7701.722	7701.732	-10.2
7	1	6	6	1	5	7876.140	7876.131	9.3

Table 12: Observed Transitions of the C3-^{13}C-substituted species

Isotopologue C4

J'	K'_a	K'_c	J	K_a	K_c	ν_{obs}[MHz]	ν_{calc}[MHz]	ν_{obs}-ν_{calc} [kHz]
3	0	3	2	0	2	3287.032	3287.035	-2.8
3	0	3	2	0	2	3287.034	3287.035	-1.0
3	0	3	2	0	2	3287.035	3287.035	-0.6
4	1	4	3	1	3	4262.418	4262.416	2.5
4	1	3	3	1	2	4507.350	4507.351	-1.1
5	1	5	4	1	4	5326.827	5326.825	2.5
5	1	4	4	1	3	5632.941	5632.936	5.2
6	1	6	5	1	5	6390.458	6390.461	-2.7
6	2	4	5	2	3	6599.070	6599.069	0.2
6	1	5	5	1	4	6757.656	6757.661	-4.5
7	1	7	6	1	6	7453.193	7453.193	0.1
7	2	5	6	2	4	7707.001	7707.001	-0.4
7	1	6	6	1	5	7881.332	7881.330	1.8

Table 13: Observed Transitions of the C4-^{13}C-substituted species

Isotopologue C5

J'	K'_a	K'_c	J	K_a	K_c	ν_{obs}[MHz]	ν_{calc}[MHz]	ν_{obs}-ν_{calc} [kHz]
3	1	2	2	1	1	3372.541	3372.552	-10.3
4	0	4	3	0	3	4366.953	4366.945	8.3
4	1	3	3	1	2	4495.941	4495.936	4.8
5	1	5	4	1	4	5309.675	5309.690	-14.8
5	0	5	4	0	4	5453.638	5453.635	3.6
5	2	3	4	2	2	5479.071	5479.082	-10.6
5	1	4	4	1	3	5618.621	5618.622	-0.4
6	1	6	5	1	5	6369.835	6369.839	-4.9
6	0	6	5	0	5	6537.001	6536.994	7.3
6	2	4	5	2	3	6581.029	6581.023	6.7
7	1	7	6	1	6	7429.055	7429.054	0.7
7	0	7	6	0	6	7616.417	7616.411	6.4
7	2	5	6	2	4	7686.237	7686.227	10.2
7	1	6	6	1	5	7861.102	7861.114	-12.2

Table 14: Observed Transitions of the C5-^{13}C-substituted species

Isotopologue C6

J'	K'_a	K'_c	J	K_a	K_c	ν_{obs}[MHz]	ν_{calc}[MHz]	ν_{obs}-ν_{calc} [kHz]
3	1	3	2	1	2	3169.067	3169.064	3.4
3	0	3	2	0	2	3257.896	3257.901	-4.8
3	1	2	2	1	1	3351.081	3351.091	-9.8
4	1	4	3	1	3	4224.681	4224.674	6.4
4	0	4	3	0	3	4340.854	4340.860	-5.5
4	2	2	3	2	1	4353.241	4353.249	-8.4
4	2	2	3	2	1	4353.241	4353.249	-8.4
4	1	3	3	1	2	4467.356	4467.357	-1.2
5	1	5	4	1	4	5279.659	5279.660	-1.4
5	0	5	4	0	4	5421.261	5421.251	10.4
5	2	3	4	2	2	5445.560	5445.575	-15.2
5	1	4	4	1	3	5582.950	5582.955	-5.1

J'	K'_a	K'_c	J	K_a	K_c	ν_{obs}[MHz]	ν_{calc}[MHz]	ν_{obs}-ν_{calc} [kHz]
6	1	6	5	1	5	6333.876	6333.881	-5.3
6	0	6	5	0	5	6498.461	6498.456	5.8
6	2	5	5	2	4	6518.069	6518.049	20.3
6	2	4	5	2	3	6540.561	6540.547	14.2
6	1	5	5	1	4	6697.694	6697.703	-9.2
7	1	7	6	1	6	7387.197	7387.206	-8.9
7	0	7	6	0	6	7571.882	7571.887	-5.3
7	2	6	6	2	5	7602.763	7602.756	6.7
7	2	5	6	2	4	7638.644	7638.644	0.7
7	1	6	6	1	5	7811.413	7811.406	7.1

Table 15: Observed Transitions of the C6-^{13}C-substituted species

Isotopologue C7

J'	K'_a	K'_c	J	K_a	K_c	ν_{obs}[MHz]	ν_{calc}[MHz]	ν_{obs}-ν_{calc} [kHz]
3	1	3	2	1	2	3162.461	3162.455	5.2
4	1	4	3	1	3	4215.888	4215.888	0.0
4	0	4	3	0	3	4330.701	4330.711	-10.4
4	1	3	3	1	2	4455.489	4455.497	-8.1
5	1	5	4	1	4	5268.704	5268.717	-13.2
5	0	5	4	0	4	5408.739	5408.728	11.2
5	2	4	4	2	3	5419.781	5419.785	-4.0
5	3	2	4	3	1	5423.361	5423.352	9.5
5	1	4	4	1	3	5568.181	5568.173	7.7
6	0	6	5	0	5	6483.671	6483.665	5.7
6	3	4	5	3	3	6508.721	6508.712	9.0
6	2	4	5	2	3	6524.341	6524.337	4.8
6	1	5	5	1	4	6680.038	6680.029	9.5
7	1	7	6	1	6	7372.030	7372.028	2.6
7	0	7	6	0	6	7554.950	7554.952	-2.0
7	2	6	6	2	5	7584.777	7584.785	-7.2
7	2	5	6	2	4	7619.462	7619.466	-4.1
7	1	6	6	1	5	7790.862	7790.875	-13.8

Table 16: Observed Transitions of the C7-^{13}C-substituted species

Isotopologue C8

J'	K'_a	K'_c	J	K_a	K_c	ν_{obs}[MHz]	ν_{calc}[MHz]	ν_{obs}-ν_{calc} [kHz]
3	1	3	2	1	2	3175.761	3175.764	-3.1
4	1	4	3	1	3	4233.581	4233.580	1.2
4	0	4	3	0	3	4351.247	4351.244	3.8
4	1	3	3	1	2	4479.621	4479.618	3.4
5	1	5	4	1	4	5290.741	5290.748	-6.5
5	3	2	4	3	1	5449.770	5449.769	0.6
5	1	4	4	1	3	5598.221	5598.232	-10.6
6	1	6	5	1	5	6347.121	6347.124	-2.5
6	0	6	5	0	5	6513.537	6513.540	-3.0
6	1	5	5	1	4	6715.961	6715.960	1.8
7	1	7	6	1	6	7402.582	7402.575	7.5
7	0	7	6	0	6	7589.122	7589.122	-0.2
7	1	6	6	1	5	7832.601	7832.597	4.2

Table 17: Observed Transitions of the C8-^{13}C-substituted species

Isotopologue C9

J'	K'_a	K'_c	J	K_a	K_c	ν_{obs}[MHz]	ν_{calc}[MHz]	ν_{obs}-ν_{calc} [kHz]
3	1	3	2	1	2	3192.441	3192.440	0.9
3	0	3	2	0	2	3282.781	3282.783	-2.7
3	1	2	2	1	1	3377.639	3377.648	-8.6
4	0	4	3	0	3	4373.918	4373.921	-2.7
4	1	3	3	1	2	4502.736	4502.737	-0.8
5	1	5	4	1	4	5318.538	5318.540	-1.4
5	0	5	4	0	4	5462.381	5462.392	-10.5
5	1	4	4	1	3	5627.123	5627.132	-9.2
6	1	6	5	1	5	6380.479	6380.472	6.9
6	1	5	5	1	4	6750.641	6750.643	-1.4
6	1	5	5	1	4	6750.641	6750.643	-1.4
7	1	7	6	1	6	7441.470	7441.476	-5.8
7	0	7	6	0	6	7628.811	7628.804	6.9
7	2	5	6	2	4	7698.122	7698.117	4.4
7	1	6	6	1	5	7873.079	7873.066	12.5

Table 18: Observed Transitions of the C9-^{13}C-substituted species