Supplementary Material

Bond Length Alternation and Internal Dynamics in Model Aromatic Substituents of Lignin

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Strong-field coherence breaking (SFCB) details

Strong-field coherence breaking (SFCB) was used in order to facilitate assignment of the intermingled transitions due to the two conformations. It was possible to identify unambiguously a set of transitions associated with each conformer. Initially, we identified a set of three transition frequencies at 10632.625, 12267.313, and 15554.375 MHz for SFCB measurements. The final SFCB measurement was recorded with a 1 μs broadband sweep followed by three 150 ns single-frequency pulses. A total of 22 transitions were identified by having their intensities modulated more than 30% compared to the 8-18 GHz sweep in the absence of the selective excitation pulses. Noting that the experimental conformer-specific transitions matched the pattern of the calculated 8-18 GHz microwave spectrum for the *syn*-4-VG, these transitions were used as a starting point for the rigid rotor fit.

For the *anti*-4VG conformer, the SFCB method was repeated for the remaining unassigned transitions using the same microwave settings. In this case, we used the line picking scheme to choose a set of resonant frequencies at 9130.875, 13415.313, 1 6373.313 MHz due to the other conformer. These transitions were subsequently assigned as the $5_{2,4}$-$4_{1,3}$, $6_{3,4}$-$5_{2,3}$, and $6_{4,3}$-$5_{3,2}$ transitions, respectively. This second set of frequencies modulated 16 transitions more than 50% relative to the original sweep taken in their absence. The line frequencies obtained through the SFCB difference spectrum were used for the initial rigid rotor fit with a standard deviation on the fit of 12 kHz.

Internal rotation methyl barrier of 4-methyl guaiacol (**MG**)

The program *XIAM* was initially used to fit the full set of transitions including internal rotation-rotation coupling. The fitted molecular parameters are summarized in Table S2. Note that in this fit some E-lines were not accurately predicted resulting in a high standard deviation. Since, the internal rotation barrier is quite low, we decided to use SPFIT, in order to obtain a better result. The obtained standard deviation with SPFIT was considerably lower (3.7 kHz). However, there are some peculiar characteristics regarding the fit that are worth mentioning. For example, when the Q-type transitions of the E-state are included, the fit required the entire set of quartic centrifugal distortion constants for the E-state and the fitted D_J is unusually big and negative (-4.256(54) kHz). Therefore, the Q-E lines have not been included in the fit in Table S2. It is worth noting that the quantum chemical calculations show excellent agreement with the experimentally deduced rotational constants.

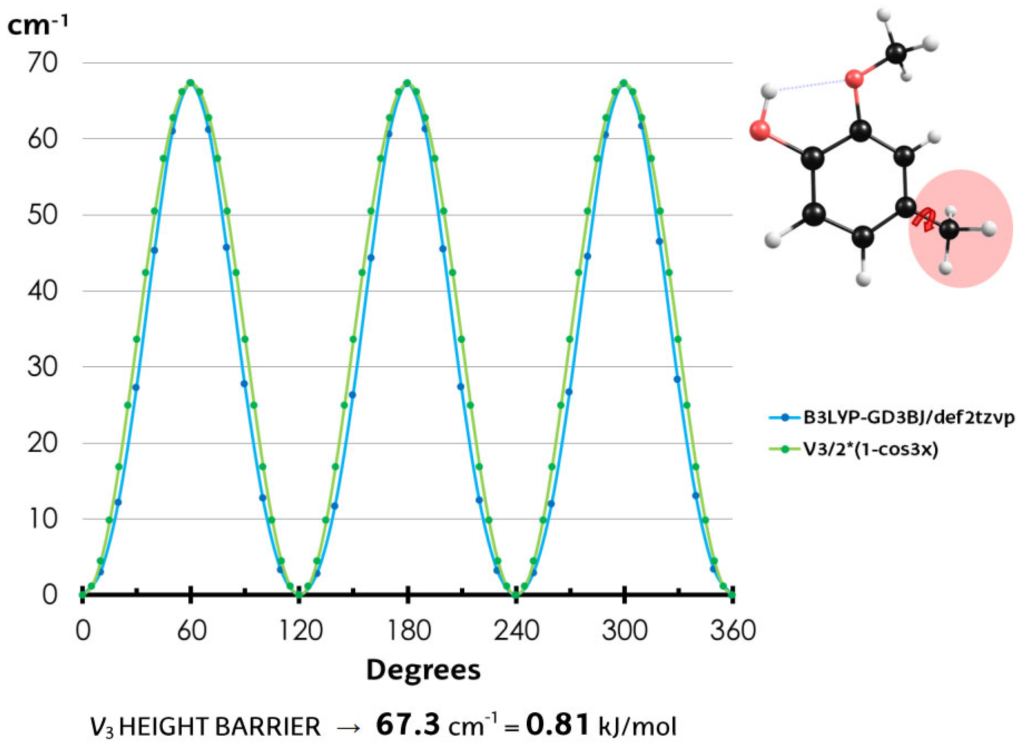

Figure S1: Experimental and simulated variation of the internal rotational barrier of methyl group.

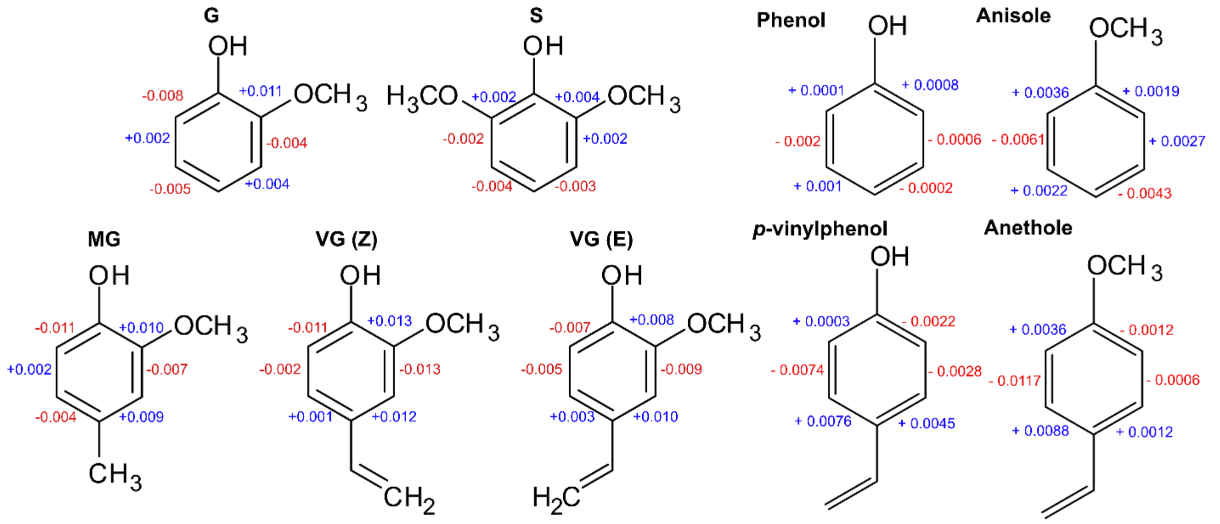

Figure S2: Summary of bond changes of lignin relative to the average bond length $r_{C\text{-}C}$. The values have been obtained from calculations at the B3LYP-GD3BJ/def2tzvp level of theory. Color coding identifies an increase in blue and a decrease in red.

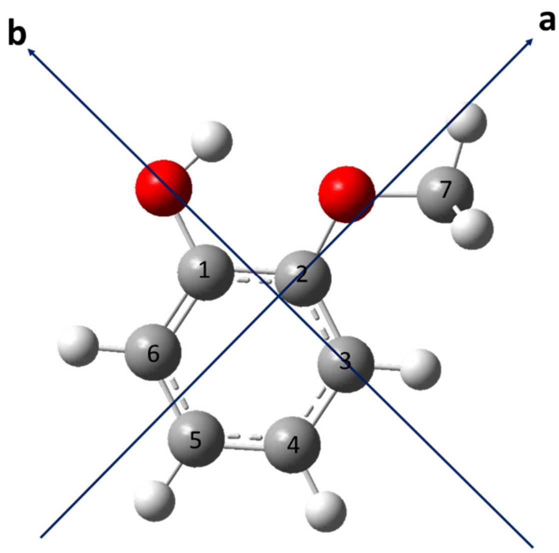

Figure S3: Optimized structure of guaiacol at B3LYP-D3BJ/def2tzvp level of theory. The atom numbering and the inertial axes have been indicated.

Table S1: Experimental and calculated constants derived from the broadband rotational spectrum of guaiacol.

	$(CH_3O)C_6H_4OH$	B3LYP-GD3BJ def2tzvp
A (MHz)	2607.06592(51)[d]	2622.1
B (MHz)	1560.79594(41)	1562.4
C (MHz)	982.87202(39)	985.2
D_J (kHz)	0.0440(42)	0.1792
D_{JK} (kHz)	0.1545(45)	-0.2532
D_K (kHz)	0.113(10)	0.0886
d_1 (kHz)	-0.01988(99)	-0.0512
d_2 (kHz)	-0.00555(39)	-0.0080
k	-0.288	-0.295
P_{aa} (uÅ^2)	322.1	321.9
P_{bb} (uÅ^2)	192.1	191.1
P_{cc} (uÅ^2)	1.7	1.6
μ_a (D)	-	-2.11
μ_b (D)	-	1.68
μ_c (D)	-	0.000
Δ (uA^2)[a]	-3.4594(2)	-3.23
σ (kHz)[b]	12.8	-
N[c]	158	-

[a] Inertial defect $\Delta I = I_c - I_b - I_a$. [b] Number of transitions in the fit. [c] Root-mean-square deviation of the fit. [d] Standard error in parentheses in units of the last digit.

Table S2: List of spectroscopic parameters used to fit guaiacol isotopomers. The centrifugal distortion constants have been fix to the values fitted for the parent species. The atoms follow the numbering label showed in red in Scheme 1.

	^{13}C(1) $(CH_3O)C_6H_4OH$	^{13}C(2) $(CH_3O)C_6H_4OH$	^{13}C(3) $(CH_3O)C_6H_4OH$
A (MHz)	2606.9431(52)[d]	2594.9253(59)	2580.0260(20)
B (MHz)	1559.8292(12)	1559.9689(13)	1560.8317(13)
C (MHz)	982.47521(69)	980.81369(66)	979.02145(54)
Δ (uA^2)[a]	-3.4616(6)	-3.4590(6)	-3.4613(4)
σ (kHz)[b]	19.18	18.78	16.66
N[c]	23	22	25

	^{13}C(4) $(CH_3O)C_6H_4OH$	^{13}C(5) $(CH_3O)C_6H_4OH$	^{13}C(6) $(CH_3O)C_6H_4OH$	^{13}C(7) $(CH_3O)C_6H_4OH$
A (MHz)	2600.0179(22)	2571.7316(16)	2602.9119(22)	2598.9874(26)
B (MHz)	1545.4636(11)	1551.2281(10)	1536.0978(12)	1525.2083(14)
C (MHz)	975.78053(49)	974.04138(41)	972.43979(52)	967.52346(71)
Δ (uA^2)[a]	-3.4604(4)	-3.4584(3)	-3.4588(4)	-3.4602(5)
σ (kHz)[b]	17.50	14.12	15.45	20.24
N[c]	29	28	27	24

[a] Inertial defect $\Delta I = I_c - I_b - I_a$. [b] Number of transitions in the fit. [c] Root-mean-square deviation of the fit. [d] Standard error in parentheses in units of the last digit.

Table S3: Experimental and calculated constants derived from the broadband rotational spectrum of syringol. The rotational constants for the two substates were constrained to the same values.

	Experimental	B3LYP-GD3BJ def2tzvp
A (MHz)	2267.07311(40)[a]	2282.2
B (MHz)	768.35079(13)	767.6
C (MHz)	578.48124(10)	578.6
κ	-0.775	-0.778
P_{aa} (uÅ^2)	654.2	655.2
P_{bb} (uÅ^2)	219.4	218.2
P_{cc} (uÅ^2)	3.5	3.2
D_J (kHz)	0.00538(47)	0.0076
D_{JK} (kHz)	0.0583(29)	0.0493
D_K (kHz)	0.058(14)	0.0677
d_1 (kHz)	-0.00175(24)	-0.0022
d_2 (kHz)	-0.000830(85)	-0.0005
ΔE_{10} (MHz)[b]	0.47569(78)	-
V_2 (cm^{-1})[c]	1975	1962
μ_a (D)	-	-1.40
μ_b (D)	-	1.57
μ_c (D)	-	0.00
Δ (uA^2)[d]	-7.0357(2)	-6.38
σ (kHz)[e]	11.9	-
N[f]	327	-

[a] Standard error in parenthesis in units of the last digit [b] energy difference between the torsional tunneling substates 0^+ and 0^- (σ=1/0, the tunneling splitting is associated with twice the energy difference (ΔE_{10}) due to the selection rules). [c] OH torsional barrier height derived from a fit to the experimental tunneling splitting based on the one-dimensional model of Meyer[23], compared to calculation (right-hand column). See text for further discussion. [d] Inertial defect $\Delta I = I_c - I_b - I_a$. [e] Root-mean-square deviation of the fit. [f] Number of transitions in the fit.

Table S4: Molecular parameters of 4-methyl guaiacol. All parameters refer to the principal axis system.

4-MG	Experimental		B3LYP-GD3BJ def2tzvp
	SPFIT[a]	XIAM	
A (MHz)	1892.95(2)[b]	1892.53(1)	1897.943
B (MHz)	1168.352(3)	1168.227(7)	1171.727
C (MHz)	729.28(1)	729.222(7)	731.098
F_0 (GHz)	154.160	153.041	161.515
κ	-0.2454	-0.2452	-0.2448
Δ (uA^2)[c]	3.278	3.302	3.129
D_J (kHz)	0.0274(63)	-	0.100
D_{JK} (kHz)	0.074(16)	-	-0.132
D_K (kHz)	0.292(26)	-	0.039
d_1 (kHz)	-0.0146(14)	-	-0.039
d_2 (kHz)	-0.00404(51)	-	-0.019
Empirical Internal-Overall Rotation Distortion Constants			
	-	2177(27)	-
	-	-192(2)	-
	-	-0.22(6)	-
Perturbation Terms			
	714.35(11)	-	-
	291.145(59)	-	-
	0.1301(13)	-	-
	0.0435(!0)	-	-
	0.229(23)	-	-
	-0.217(13)	-	-
	0.00040(25)	-	-
	0.00434(27)	-	-
μ_a (D)	-	-	0.296
μ_b (D)	-	-	-2.829
μ_c (D)	-	-	0.00
V_3 (GHz)	1919.1/2221.9[d]	2198.2(3)	2018
V_3 (cm^{-1})	63.9/74.0[d]	73.32(1)	67
σ (kHz)[e]	3.71	721.2	-
N_A/N_E[f]	134/39	139/39	-

[a] Averaged values according to the following equations: $A = \frac{1}{3}(A_A + 2A_E); B = \frac{1}{3}(B_A + 2B_E); C = \frac{1}{3}(C_A + 2C_E)$. [b] Standard error in parentheses in units of the last digit. [c] Inertial defect $\Delta I = I_c - I_b - I_a$. [d] Values refer to the dimensionless perturbation first-order $W^{(1)}_{\upsilon=0}$ and second order $W^{(2)}_{\upsilon=0}$ coefficients for the three-fold barrier. [e] Root-mean-square deviation of the fit. [f] Number of A and E symmetry lines (N_A/N_E).

Table S5: Molecular parameters for *Z*- and *E*-4-vinyl guaiacol.

4-VG	*Z*		*E*	
	Experimental	**Calculated**	**Experimental**	**Calculated**
A (MHz)	1646.75211(75)[a]	1652.1596	1867.7943(12)	1874.2983
B (MHz)	872.49030(47)	874.3385	779.97187(44)	781.7989
C (MHz)	572.90499(30)	573.8423	552.77983(47)	553.6226
D_J (kHz)	0.0185(19)	0.02096	0.0077(18)	0.01160
D_K (kHz)	0.085(19)	0.08358	-	0.16252
D_{JK} (kHz)	-	0.01149	0.148(26)	0.03534
d_1 (kHz)	-0.00693(95)	7.69×10^{-3}	-	3.75×10^{-3}
d_2 (kHz)	-	0.04726	-	0.04467
μ_a (D)	-	0.347	-	-0.979
μ_b (D)	-	2.400	-	2.475
μ_c (D)	-	0.000	-	0.000
ΔE_{rel} (cm^{-1})	-	0	-	136
%[b]	75(3)	60.4	24(4)	39.6
Δ (uA^2)[c]	-3.9977(6)	-3.21	-4.2703(9)	-3.21
σ (kHz)[d]	14	-	12	-
N[e]	81	-	45	-

[a] Standard error in parenthesis in units of the last digit [b] Boltzmann distribution. [c] Inertial defect $\Delta I = I_c - I_b - I_a$. [d] Root-mean-square deviation of the fit. [e] Number of transitions in the fit.

Table S6: Line list of transitions fitted for guaiacol (**G**).

		Frequency	error
3 1 3	2 1 2	6664.0417	0.0002
3 3 1	3 2 2	6776.2111	-0.0044
7 4 3	7 3 4	6782.8982	0.0025
9 4 5	9 3 6	6785.0860	-0.0039
3 0 3	2 0 2	6998.4662	-0.0002
4 2 3	4 1 4	7127.8079	-0.0100
3 1 3	2 0 2	7313.8263	-0.0024
8 3 5	8 2 6	7340.1748	-0.0022
6 4 2	6 3 3	7578.5916	-0.0079
3 2 2	2 2 1	7630.9949	-0.0010
5 1 4	5 1 5	7798.2326	0.0108
5 1 4	5 0 5	7844.1504	-0.0012
5 3 3	5 2 4	7930.5147	-0.0005
10 5 5	10 4 6	8038.3531	0.0094
3 2 1	2 2 0	8263.5229	-0.0047
3 1 2	2 1 1	8360.0303	-0.0030
5 4 1	5 3 2	8367.0467	0.0045
4 1 3	3 2 2	8433.6153	-0.0058
6 3 3	5 4 2	8498.6035	0.0054
4 0 4	3 1 3	8614.3943	-0.0016
7 2 5	7 2 6	8651.2902	-0.0074
5 2 4	5 1 5	8683.4316	-0.0017
5 2 4	5 0 5	8729.3645	0.0013
4 1 4	3 1 3	8741.7590	-0.0010
4 3 2	4 1 3	8794.2994	-0.0010
2 2 1	1 1 0	8804.0622	-0.0012
5 3 3	5 1 4	8815.7274	0.0006
9 5 4	9 4 5	8817.7032	0.0124
7 2 5	7 1 6	8822.0673	-0.0040
12 5 7	12 4 8	8843.8055	0.0042
4 4 0	4 3 1	8872.6965	-0.0025
4 0 4	3 0 3	8929.7584	0.0001
5 2 3	4 3 2	8997.6651	-0.0090
6 3 4	6 2 5	9001.2667	0.0133
4 1 4	3 0 3	9057.1212	-0.0011
4 4 1	4 3 2	9114.0601	-0.0024
5 4 2	5 3 3	9180.8217	-0.0060
3 3 1	3 1 2	9185.9804	-0.0039
6 3 4	6 1 5	9415.5301	-0.0106
6 4 3	6 3 4	9432.8543	-0.0047
2 2 0	1 1 1	9563.4290	0.0003
9 3 6	9 2 7	9575.2912	-0.0174
8 5 3	8 4 4	9867.0606	0.0010
12 6 6	12 5 7	9882.2453	-0.0569
7 4 4	7 3 5	9964.2713	0.0015
6 1 5	6 0 6	10028.6136	0.0029
4 2 3	3 2 2	10030.0470	0.0001
7 3 5	7 2 6	10385.4757	0.0028
6 2 5	6 1 6	10427.4507	-0.0001
6 2 5	6 0 6	10442.9299	0.0319
4 3 2	3 3 1	10451.7063	0.0002
4 3 1	3 3 0	10661.7612	-0.0004
5 0 5	4 1 4	10717.0557	0.0000
7 5 2	7 4 3	10761.0374	0.0016
5 1 5	4 1 4	10762.9843	-0.0012
3 2 2	2 1 1	10769.8002	-0.0020
8 4 5	8 3 6	10832.5630	0.0000
4 1 3	3 1 2	10843.3899	0.0000
5 0 5	4 0 4	10844.4206	0.0008
5 1 5	4 0 4	10890.3133	-0.0362

		Frequency	error
11 6 5	11 5 6	11013.9895	-0.0634
8 2 6	8 2 7	11111.7633	-0.0069
8 2 6	8 1 7	11176.3921	-0.0020
4 2 2	3 2 1	11268.4728	-0.0062
6 5 1	6 4 2	11316.7713	-0.0056
5 1 4	4 2 3	11433.3899	0.0005
7 5 3	7 4 4	11528.2113	-0.0034
6 5 2	6 4 3	11564.4193	-0.0059
5 5 0	5 4 1	11595.4494	-0.0052
8 5 4	8 4 5	11633.9780	0.0189
5 5 1	5 4 2	11650.2706	-0.0031
9 5 5	9 4 6	11983.6776	0.0010
8 3 6	8 2 7	12017.4384	0.0048
7 1 6	7 0 7	12117.1827	0.0009
10 6 4	10 5 5	12232.4318	-0.0020
6 4 3	6 2 4	12280.4116	-0.0127
7 2 6	7 1 7	12282.9925	-0.0038
7 2 6	7 0 7	12287.9459	-0.0095
5 2 4	4 2 3	12318.6005	-0.0003
4 2 3	3 1 2	12439.8130	-0.0028
7 3 4	6 4 3	12542.3678	-0.0109
10 5 6	10 4 7	12656.7356	0.0088
6 2 4	5 3 3	12719.3192	-0.0030
6 0 6	5 1 5	12736.6860	0.0012
6 1 6	5 1 5	12752.1333	0.0013
6 0 6	5 0 5	12782.6169	0.0022
6 1 6	5 0 5	12798.0619	0.0001
5 1 4	4 1 3	13029.8163	0.0011
5 3 3	4 3 2	13051.2417	0.0002
5 4 2	4 4 1	13118.0074	0.0008
5 4 1	4 4 0	13167.3574	0.0009

		Frequency	error
9 6 3	9 5 4	13169.9268	0.0029
3 2 1	2 1 2	13317.5439	-0.0017
9 2 7	9 2 8	13400.9127	0.0009
9 2 7	9 1 8	13424.0097	0.0441
10 4 7	10 3 8	13548.2592	-0.0019
5 3 2	4 3 1	13673.0131	-0.0002
11 5 7	11 4 8	13685.4199	-0.0106
8 6 2	8 5 3	13746.7824	0.0065
9 3 7	9 2 8	13815.2939	-0.0029
10 6 5	10 5 6	13828.1965	0.0077
9 3 7	9 1 8	13838.3318	-0.0188
9 6 4	9 5 5	13849.7796	0.0015
5 2 4	4 1 3	13915.0248	-0.0018
8 6 3	8 5 4	13975.2629	0.0051
11 6 6	11 5 7	14012.6779	0.0520
7 6 1	7 5 2	14064.5610	-0.0047
6 1 5	5 2 4	14081.8614	-0.0007
7 6 2	7 5 3	14123.2087	-0.0043
8 1 7	8 1 8	14129.5010	0.0031
8 1 7	8 0 8	14131.0435	0.0056
5 2 3	4 2 2	14143.1422	-0.0014
8 2 7	8 1 8	14194.1223	0.0005
3 3 1	2 2 0	14225.7689	-0.0012
6 6 0	6 5 1	14237.0460	0.0295
6 6 1	6 5 2	14247.4917	-0.0106
3 3 0	2 2 1	14444.9860	-0.0008
6 2 5	5 2 4	14496.1485	-0.0009
12 6 7	12 5 8	14497.0839	0.0168
11 3 8	11 2 9	14516.8634	-0.0176
12 7 5	12 6 6	14645.5135	0.0312
7 0 7	6 1 6	14721.4903	0.0043

		Frequency	error
7 1 7	6 1 6	14726.4443	-0.0008
7 0 7	6 0 6	14736.9410	0.0079
7 1 7	6 0 6	14741.9033	0.0110
6 1 5	5 1 4	14967.0768	0.0031
12 5 8	12 4 9	15047.7306	-0.0192
11 4 8	11 3 9	15272.7198	-0.0125
6 2 5	5 1 4	15381.3638	0.0028
10 2 8	10 2 9	15534.7312	-0.0017
10 2 8	10 1 9	15542.6012	-0.0082
6 3 4	5 3 3	15566.8879	0.0002
11 7 4	11 6 5	15582.8680	0.0417
10 3 8	10 2 9	15706.8890	0.0096
10 3 8	10 1 9	15714.7629	0.0068
6 5 2	5 5 1	15733.0996	0.0292
6 5 1	5 5 0	15742.7037	0.0011
15 8 7	15 7 8	15759.8947	-0.0070
6 4 3	5 4 2	15818.9190	0.0000
9 4 5	8 5 4	15873.1128	-0.0182

		Frequency	error
6 4 2	5 4 1	16021.3933	0.0130
9 2 8	9 1 9	16128.5864	-0.0003
7 2 5	6 3 4	16232.0324	-0.0024
7 1 6	6 2 5	16411.2219	0.0050
4 3 2	3 2 1	16413.9540	0.0054
9 7 3	9 6 4	16565.5546	-0.0142
7 2 6	6 2 5	16581.9914	0.0008
8 0 8	7 1 7	16693.3595	0.0000
8 1 8	7 1 7	16694.9013	0.0017
8 0 8	7 0 7	16698.3164	-0.0022
8 1 8	7 0 7	16699.8612	0.0025
8 7 2	8 6 3	16733.4942	-0.0350
6 2 4	5 2 3	16772.8918	0.0023
6 3 3	5 3 2	16809.8233	0.0005
7 1 6	6 1 5	16825.5053	0.0011
7 2 6	6 1 5	16996.2819	0.0039
4 3 1	3 2 2	17475.7523	-0.0002
4 2 2	3 1 3	17921.9825	-0.0007

Table S8: Line list of transitions fitted for ^{13}C(2) guaiacol.

		Frequency	error
4 0 4	3 0 3	8909.7556	-0.0135
6 0 6	5 0 5	12755.3154	0.0046
3 1 2	2 1 1	8351.2478	-0.0446
4 1 4	3 1 3	8725.1466	-0.0126
4 3 1	3 3 0	10657.1994	0.0071
4 1 3	3 1 2	10827.3576	0.0186
4 2 2	3 2 1	11263.4300	0.0237
5 2 4	4 2 3	12299.5332	-0.0268
6 1 6	5 1 5	12725.9000	0.0008
6 0 6	5 1 5	12711.1631	-0.0082
6 1 6	5 0 5	12770.0140	-0.0245

		Frequency	error
5 1 4	4 1 3	13003.6482	0.0134
5 4 2	4 4 1	13108.2049	0.0112
5 2 3	4 2 2	14131.8152	-0.0188
6 2 5	5 2 4	14470.7538	0.0097
7 0 7	6 1 6	14691.1261	0.0038
7 1 7	6 1 6	14695.8159	0.0024
6 1 5	5 1 4	14932.4164	-0.0128
5 0 5	4 1 4	10697.3159	0.0336
2 2 0	1 1 1	9528.3097	0.0041
4 1 4	3 0 3	9033.1853	0.0304
3 1 3	2 0 2	7291.8221	-0.0045

Table S9: Line list of transitions fitted for ^{13}C(3) guaiacol.

		Frequency	error
3 1 3	2 1 2	6643.8623	-0.0204
3 0 3	2 0 2	6970.9879	-0.0080
3 1 2	2 1 1	8349.2968	0.0051
4 0 4	3 1 3	8594.1211	0.0171
4 1 4	3 1 3	8711.7601	0.0019
2 2 1	1 1 0	8719.0838	-0.0093
4 0 4	3 0 3	8891.4706	-0.0081
3 1 3	2 0 2	7268.3601	-0.0106
4 2 3	3 2 2	10010.1113	0.0168
4 3 1	3 3 0	10664.9561	-0.0238
3 2 2	2 1 1	10677.1271	-0.0037
4 1 3	3 1 2	10817.3812	-0.0449
4 2 2	3 2 1	11270.9801	0.0017

		Frequency	error
6 0 6	5 1 5	12689.6075	-0.0020
6 1 6	5 1 5	12703.2817	-0.0309
6 1 6	5 0 5	12744.8771	-0.0075
5 1 4	4 1 3	12981.1849	0.0170
3 3 1	2 2 0	14085.8938	0.0084
5 2 3	4 2 2	14133.6443	0.0209
3 3 0	2 2 1	14313.0018	-0.0051
7 0 7	6 1 6	14664.9187	-0.0029
7 0 7	6 0 6	14678.6461	0.0214
7 1 7	6 0 6	14682.9425	0.0055
6 1 5	5 1 4	14899.9102	0.0251
6 2 5	5 1 4	15278.2214	0.0020

Table S10: Line list of transitions fitted for ^{13}C(4) guaiacol.

		Frequency	error
3 1 3	2 1 2	6611.9868	-0.0224
3 0 3	2 0 2	6947.9923	-0.0290
3 1 3	2 0 2	7272.8287	0.0002
4 1 4	3 1 3	8675.8811	0.0099
4 1 4	3 0 3	9000.6550	-0.0232
4 2 3	3 2 2	9944.8425	0.0018
2 2 1	1 1 0	8775.8439	0.0157
2 2 0	1 1 1	9521.4688	0.0095
4 3 2	3 3 1	10354.6922	0.0057
5 0 5	4 1 4	10635.1747	0.0294
5 1 5	4 1 4	10683.7523	-0.0149
4 1 3	3 1 2	10754.0441	0.0187
5 0 5	4 0 4	10768.1169	-0.0269
5 1 4	4 2 3	11300.9541	0.0121
5 2 4	4 2 3	12218.4632	-0.0097
6 0 6	5 1 5	12642.8929	0.0316
6 1 6	5 1 5	12659.4538	0.0179
6 0 6	5 0 5	12691.4743	-0.0089
6 1 6	5 0 5	12708.0780	0.0202
5 1 4	4 1 3	12934.0585	0.0034
3 2 1	2 1 2	13228.0601	-0.0254
5 3 2	4 3 1	13529.6122	-0.0186
5 2 4	4 1 3	13851.5798	-0.0062
5 2 3	4 2 2	14010.3098	0.0146
3 3 1	2 2 0	14181.9405	0.0068
7 0 7	6 1 6	14614.5702	-0.0063
7 0 7	6 0 6	14631.1219	-0.0291
7 1 7	6 0 6	14636.5537	0.0097
6 2 5	5 1 4	15300.9039	0.0008

Table S11: Line list of transitions fitted for ^{13}C(5) guaiacol.

		Frequency	error
3 1 3	2 1 2	6608.4806	-0.0242
3 0 3	2 0 2	6935.6746	-0.0067
4 0 4	3 1 3	8546.7883	0.0221
4 1 4	3 1 3	8666.3485	-0.0054
4 0 4	3 0 3	8847.2698	-0.0076
2 2 1	1 1 0	8689.2157	-0.0143
2 2 0	1 1 1	9450.7933	0.0054
4 2 3	3 2 2	9953.9967	0.0053
4 3 2	3 3 1	10381.3921	-0.0070
5 0 5	4 1 4	10625.6001	-0.0055
3 2 2	2 1 1	10637.3331	0.0255
5 1 5	4 0 4	10787.6919	-0.0006
4 2 2	3 2 1	11200.9545	0.0061
5 2 4	4 2 3	12220.2850	0.0037
6 0 6	5 1 5	12624.3916	0.0035
6 1 6	5 1 5	12638.4644	-0.0119
6 0 6	5 0 5	12666.8793	-0.0077
6 1 6	5 0 5	12680.9492	-0.0263
5 1 4	4 1 3	12914.8877	0.0136
5 3 3	4 3 2	12960.8271	-0.0124
5 3 2	4 3 1	13598.9062	-0.0037
3 3 1	2 2 0	14038.4046	-0.0121
3 3 0	2 2 1	14261.9223	-0.0016
7 1 7	6 1 6	14594.5625	-0.0159
7 0 7	6 0 6	14604.2186	0.0104
7 1 7	6 0 6	14608.6983	0.0315
6 1 5	5 1 4	14826.8537	0.0231
6 2 5	5 1 4	15212.6444	-0.0031

Table S12: Line list of transitions fitted for ^{13}C(6) guaiacol.

		Frequency	error
3 1 3	2 1 2	6585.4112	0.0345
4 1 4	3 1 3	8643.2786	0.0066
2 2 1	1 1 0	8781.1590	-0.0102
4 0 4	3 0 3	8839.6018	0.0047
2 2 0	1 1 1	9516.0612	-0.0127
4 2 3	3 2 2	9897.8541	-0.0089
3 1 2	2 1 1	8241.9800	0.0060
3 2 1	2 2 0	8127.0678	-0.0173
4 3 2	3 3 1	10297.6966	0.0133
5 1 5	4 1 4	10645.5340	-0.0055
4 1 3	3 1 2	10705.7198	0.0149
5 0 5	4 0 4	10733.2495	0.0133
5 1 5	4 0 4	10784.8684	0.0016
5 2 4	4 2 3	12165.1523	-0.0430
6 0 6	5 1 5	12597.5002	0.0080
6 1 6	5 1 5	12615.3305	0.0015
6 0 6	5 0 5	12649.1107	-0.0119
5 3 3	4 3 2	12863.4894	0.0043
5 1 4	4 1 3	12887.4283	-0.0149
5 2 4	4 1 3	13841.4266	0.0035
6 1 5	5 2 4	13865.7835	0.0129
3 3 1	2 2 0	14192.3187	0.0168
6 2 5	5 2 4	14325.6349	-0.0263
7 0 7	6 1 6	14563.7538	0.0049
7 0 7	6 0 6	14581.5782	-0.0075
6 1 5	5 1 4	14819.7514	0.0012
6 3 4	5 3 3	15352.3830	0.0187

Table S13: Line list of transitions fitted for $^{13}C(7)$ guaiacol.

		Frequency	error
3 1 3	2 1 2	6549.0034	0.0000
2 2 1	1 1 0	8764.5073	0.0279
4 1 3	3 1 2	10642.5678	-0.0237
4 2 2	3 2 1	11006.7218	-0.0035
5 1 4	4 1 3	12820.2417	-0.0170
6 1 6	5 0 5	12604.8908	-0.0012
6 0 6	5 0 5	12586.0693	0.0029
6 0 6	5 1 5	12532.1265	-0.0039
4 2 2	3 2 1	11006.7218	-0.0035
4 1 3	3 1 2	10642.5678	-0.0237
4 1 4	3 1 3	8597.3299	0.0028
4 1 4	3 0 3	8940.7212	0.0087

		Frequency	error
4 2 3	3 2 2	9837.9343	0.0589
4 3 1	3 3 0	10414.5776	-0.0152
5 0 5	4 1 4	10536.5021	0.0055
5 1 5	4 0 4	10734.4933	0.0218
6 1 6	5 1 5	12550.9376	-0.0186
5 3 3	4 3 2	12779.5078	0.0004
5 2 4	4 1 3	13800.7067	0.0146
3 3 1	2 2 0	14166.6423	-0.0189
6 2 5	5 2 4	14246.6300	-0.0089
3 3 0	2 2 1	14367.0385	-0.0031
7 0 7	6 0 6	14508.2872	-0.0258
6 3 4	5 3 3	15255.6655	0.0401

Table S14: Line list of transitions fitted for syringol (**S**).

				Frequency	error
3 1 2	0	3 0 3	0	2235.8987	-0.0063
2 1 2	0	1 1 1	1	2503.2941	-0.0243
2 1 2	1	1 1 1	0	2504.2770	0.0071
3 0 3	0	2 1 2	0	2647.9136	0.0002
2 0 2	0	1 0 1	1	2676.2717	0.0044
2 0 2	1	1 0 1	0	2677.2156	-0.0029
4 1 3	0	4 0 4	0	2740.4975	0.0009
1 1 1	0	0 0 0	0	2845.5550	0.0007
2 1 1	0	1 1 0	1	2883.0466	-0.0108
2 1 1	1	1 1 0	0	2884.0018	-0.0070
5 1 4	0	4 2 3	0	3258.1238	0.0046
5 1 4	0	5 0 5	0	3435.0357	0.0006
3 1 3	0	2 1 2	1	3745.0768	0.0039
3 1 3	1	2 1 2	0	3746.0174	-0.0069
3 0 3	0	2 0 2	1	3973.2107	-0.0003
3 0 3	1	2 0 2	0	3974.1631	0.0005
5 2 3	0	5 1 4	0	3987.7063	0.0049
6 2 4	0	6 1 5	0	3988.1811	0.0028
2 1 2	0	1 0 1	0	4002.5177	0.0014
3 2 2	0	2 2 1	1	4040.0220	0.0034
3 2 2	1	2 2 1	0	4040.9585	-0.0113
3 2 1	0	2 2 0	1	4106.8329	0.0058
3 2 1	1	2 2 0	0	4107.7918	0.0132
4 2 2	0	4 1 3	0	4111.7330	0.0027
4 0 4	0	3 1 3	0	4128.0031	-0.0007
7 2 5	0	7 1 6	0	4156.8576	0.0063
3 2 1	0	3 1 2	0	4306.1767	-0.0023
3 1 2	0	2 1 1	1	4313.7307	-0.0034
3 1 2	1	2 1 1	0	4314.6885	0.0029
6 1 5	0	6 0 6	0	4327.1766	0.0039

				Frequency	error
2 2 0	0	2 1 1	0	4513.0859	-0.0001
8 2 6	0	8 1 7	0	4527.0571	0.0003
4 1 4	0	3 1 3	1	4975.9272	-0.0028
4 1 4	1	3 1 3	0	4976.8825	0.0011
6 1 5	0	5 2 4	0	5049.7109	-0.0011
2 2 1	0	2 1 2	0	5065.7737	0.0000
3 1 3	0	2 0 2	0	5071.3217	-0.0002
9 2 7	0	9 1 8	0	5122.1996	0.0114
4 0 4	0	3 0 3	1	5225.1710	0.0076
4 0 4	1	3 0 3	0	5226.1239	0.0091
3 2 2	0	3 1 3	0	5360.7218	0.0024
4 2 3	0	3 2 2	1	5373.6613	-0.0015
4 2 3	1	3 2 2	0	5374.6170	0.0027
7 1 6	0	7 0 7	0	5398.0360	0.0057
4 3 2	0	3 3 1	1	5418.0295	0.0006
4 3 2	1	3 3 1	0	5418.9771	-0.0031
4 3 1	0	3 3 0	1	5423.6884	0.0070
4 3 1	1	3 3 0	0	5424.6479	0.0152
4 2 2	0	3 2 1	1	5535.3070	0.0007
4 2 2	1	3 2 1	0	5536.2611	0.0035
5 0 5	0	4 1 4	0	5581.5371	0.0009
4 1 3	0	3 1 2	1	5729.7577	0.0028
4 1 3	1	3 1 2	0	5730.7136	0.0072
4 2 3	0	4 1 4	0	5758.4569	0.0047
10 2 8	0	10 1 9	0	5950.7831	0.0001
11 3 8	0	11 2 9	0	6044.6949	-0.0103
10 3 7	0	10 2 8	0	6063.1893	-0.0015
4 1 4	0	3 0 3	0	6074.0423	0.0014
5 1 5	0	4 1 4	1	6194.2225	0.0008
5 1 5	1	4 1 4	0	6195.1757	0.0026

				Frequency	error
5 2 4	0	5 1 5	0	6260.3437	0.0096
5 0 5	0	4 0 4	1	6429.4604	-0.0018
5 0 5	1	4 0 4	0	6430.4079	-0.0058
8 3 5	0	8 2 6	0	6577.2517	-0.0021
8 1 7	0	8 0 8	0	6604.9220	-0.0034
5 2 4	0	4 2 3	1	6696.0988	-0.0047
5 2 4	1	4 2 3	0	6697.0506	-0.0043
5 3 3	0	4 3 2	1	6782.5476	0.0037
5 3 3	1	4 3 2	0	6783.4928	-0.0023
5 3 2	0	4 3 1	1	6802.1215	0.0128
5 3 2	1	4 3 1	0	6803.0484	-0.0116
7 1 6	0	6 2 5	0	6855.8557	0.0023
6 2 5	0	6 1 6	0	6865.5184	0.0004
7 3 4	0	7 2 5	0	6945.3061	0.0027
6 0 6	0	5 1 5	0	6982.8813	0.0080
11 2 9	0	11 1 10	0	6998.9052	-0.0015
5 2 3	1	4 2 2	0	7000.9263	0.0029
5 1 5	0	4 0 4	0	7043.1013	0.0021
6 3 3	0	6 2 4	0	7298.4218	-0.0124
2 2 1	0	1 1 0	0	7379.7029	0.0045
6 1 6	0	5 1 5	1	7399.6047	0.0004
6 1 6	1	5 1 5	0	7400.5496	-0.0059
7 2 6	0	7 1 7	0	7570.0944	-0.0011
5 3 2	0	5 2 3	0	7586.1755	0.0257
2 2 0	0	1 1 1	0	7586.4839	-0.0048
6 0 6	0	5 0 5	1	7595.5598	0.0010
6 0 6	1	5 0 5	0	7596.5066	-0.0035
4 3 1	0	4 2 2	0	7783.9936	-0.0195
3 3 0	0	3 2 1	0	7895.6543	0.0162
3 3 1	0	3 2 2	0	7978.4103	-0.0102
6 2 5	0	5 2 4	1	8004.7910	0.0028

				Frequency	error
6 2 5	1	5 2 4	0	8005.7510	0.0114
6 1 6	0	5 0 5	0	8013.2370	-0.0039
4 3 2	0	4 2 3	0	8022.7810	-0.0056
5 3 3	0	5 2 4	0	8109.2235	-0.0033
6 5 1	0	5 5 0	1	8122.9755	0.0112
6 4 3	0	5 4 2	1	8137.5305	-0.0123
6 4 3	1	5 4 2	0	8138.4958	0.0015
6 4 2	0	5 4 1	1	8139.0988	-0.0107
6 4 2	1	5 4 1	0	8140.0405	-0.0204
6 3 4	0	5 3 3	1	8149.3564	0.0024
6 3 4	1	5 3 3	0	8150.3152	0.0099
6 3 3	0	5 3 2	1	8200.4740	0.0163
12 2 10	0	12 1 11	0	8227.4554	-0.0271
6 3 4	0	6 2 5	0	8253.7643	-0.0282
7 0 7	0	6 1 6	0	8323.3416	0.0003
8 2 7	0	8 1 8	0	8366.8008	0.0061
7 3 5	0	7 2 6	0	8471.7722	-0.0046
6 1 5	0	5 1 4	1	8487.6938	-0.0025
6 2 4	0	5 2 3	1	8488.1778	0.0046
6 1 5	1	5 1 4	0	8488.6498	0.0020
6 2 4	1	5 2 3	0	8489.1307	0.0061
3 2 2	0	2 1 1	0	8536.6556	-0.0037
13 4 9	0	13 3 10	0	8592.1474	-0.0002
7 1 7	0	6 1 6	1	8592.9231	-0.0058
7 1 7	1	6 1 6	0	8593.8749	-0.0055
8 1 7	0	7 2 6	0	8643.0511	-0.0212
7 0 7	0	6 0 6	1	8740.0695	-0.0026
7 0 7	1	6 0 6	0	8741.0168	-0.0066
8 3 6	0	8 2 7	0	8776.3336	-0.0077
10 2 8	0	9 3 7	0	8796.5515	0.0031
7 1 7	0	6 0 6	0	9010.6032	-0.0081

				Frequency	error
12 4 8	0	12 3 9	0	9083.0832	-0.0117
9 3 7	0	9 2 8	0	9177.4007	-0.0168
3 2 1	0	2 1 2	0	9189.9966	-0.0008
10 1 9	0	10 0 10	0	9208.8550	-0.0012
9 2 8	0	9 1 9	0	9245.3310	-0.0046
7 2 6	0	6 2 5	1	9297.5041	-0.0024
7 2 6	1	6 2 5	0	9298.4538	-0.0041
7 5 3	0	6 5 2	1	9487.5981	0.0263
7 5 3	1	6 5 2	0	9488.5040	-0.0190
7 5 2	1	6 5 1	0	9488.6247	0.0009
7 4 4	0	6 4 3	1	9509.6118	0.0027
7 4 4	1	6 4 3	0	9510.5591	-0.0013
7 4 3	0	6 4 2	1	9514.7722	-0.0067
7 3 5	0	6 3 4	1	9515.4921	0.0013
7 4 3	1	6 4 2	0	9515.7390	0.0086
7 3 5	1	6 3 4	0	9516.4433	0.0011
13 2 11	0	13 1 12	0	9578.7305	0.0165
4 2 3	0	3 1 2	0	9596.5858	-0.0021
11 4 7	0	11 3 8	0	9597.2032	0.0046
8 0 8	0	7 1 7	0	9608.2383	-0.0042
7 3 4	0	6 3 3	1	9626.4701	-0.0016
7 3 4	1	6 3 3	0	9627.4254	0.0022
10 3 8	0	10 2 9	0	9680.9339	0.0059
8 1 8	0	7 1 7	1	9775.8900	-0.0070
8 1 8	1	7 1 7	0	9776.8396	-0.0087
7 1 6	0	6 1 5	1	9810.9282	-0.0014
7 1 6	1	6 1 5	0	9811.8812	0.0002
8 0 8	0	7 0 7	1	9877.8373	0.0069
8 0 8	1	7 0 7	0	9878.7838	0.0021
7 2 5	0	6 2 4	1	9979.6039	0.0013
7 2 5	1	6 2 4	0	9980.5575	0.0034

				Frequency	error
8 1 8	0	7 0 7	0	10046.4524	0.0161
10 2 9	0	10 1 10	0	10193.3461	-0.0074
11 3 9	0	11 2 10	0	10288.3544	0.0031
9 1 8	0	8 2 7	0	10375.5063	0.0015
9 4 5	0	9 3 6	0	10451.4290	-0.0009
11 1 10	0	11 0 11	0	10514.5911	-0.0037
5 2 4	0	4 1 3	0	10562.9433	0.0066
8 2 7	0	7 2 6	1	10572.6076	0.0114
8 2 7	1	7 2 6	0	10573.5640	0.0165
8 4 4	0	8 3 5	0	10731.8687	0.0149
9 0 9	0	8 1 8	0	10849.5130	0.0174
8 3 6	0	7 3 5	1	10877.1638	0.0032
8 3 6	1	7 3 5	0	10878.1121	0.0001
8 4 5	0	7 4 4	1	10887.4008	-0.0015
11 2 9	0	10 3 8	0	10888.3517	0.0228
8 4 5	1	7 4 4	0	10888.3517	-0.0019
8 4 4	0	7 4 3	1	10901.3984	0.0005
8 4 4	1	7 4 3	0	10902.3528	0.0036
7 4 3	0	7 3 4	0	10917.3507	0.0132
9 1 9	0	8 1 8	1	10950.6136	0.0003
9 1 9	1	8 1 8	0	10951.5601	-0.0045
4 2 2	0	3 1 3	0	10980.2328	0.0021
12 3 10	0	12 2 11	0	10996.6857	0.0111
9 0 9	0	8 0 8	1	11017.1533	0.0032
9 0 9	1	8 0 8	0	11018.1012	-0.0001
6 4 2	0	6 3 3	0	11029.0329	0.0026
8 1 7	0	7 1 6	1	11084.7286	0.0031
8 1 7	1	7 1 6	0	11085.6740	-0.0028
8 3 5	0	7 3 4	1	11086.8789	-0.0025
8 3 5	1	7 3 4	0	11087.8379	0.0050
5 4 1	0	5 3 2	0	11090.3864	0.0080

				Frequency	error
7 4 4	0	7 3 5	0	11098.4533	-0.0023
6 4 3	0	6 3 4	0	11104.3285	-0.0088
8 4 5	0	8 3 6	0	11108.6985	0.0011
5 4 2	0	5 3 3	0	11116.1339	-0.0145
9 1 9	0	8 0 8	0	11119.2190	0.0000
4 4 0	0	4 3 1	0	11120.9037	0.0157
4 4 1	0	4 3 2	0	11127.4562	0.0127
9 4 6	0	9 3 7	0	11148.5807	0.0047
11 2 10	0	11 1 11	0	11197.6281	-0.0052
10 4 7	0	10 3 8	0	11233.8611	0.0059
11 4 8	0	11 3 9	0	11381.0615	0.0044
6 2 5	0	5 1 4	0	11443.7271	0.0032
8 2 6	0	7 2 5	1	11454.9226	-0.0083
12 4 9	0	12 3 10	0	11605.8491	0.0148
12 1 11	0	12 0 12	0	11790.3484	-0.0157
13 3 11	0	13 2 12	0	11798.7939	0.0139
9 2 8	0	8 2 7	1	11829.1593	0.0049
9 2 8	1	8 2 7	0	11830.1100	0.0043
13 4 10	0	13 3 11	0	11921.4894	0.0243
3 3 1	0	2 2 0	0	12001.9896	-0.0041
3 3 0	0	2 2 1	0	12019.8681	0.0063
10 0 10	0	9 1 9	0	12059.6615	-0.0008
10 1 10	0	9 1 9	1	12119.2120	0.0312
10 1 10	1	9 1 9	0	12120.1386	0.0065
10 0 10	0	9 0 9	1	12160.8127	0.0326
10 0 10	1	9 0 9	0	12161.7457	0.0142
10 1 10	0	9 0 9	0	12221.2456	-0.0041
9 3 7	0	8 3 6	1	12230.2322	0.0016
9 3 7	1	8 3 6	0	12231.1916	0.0096
7 2 6	0	6 1 5	0	12253.5000	-0.0340
9 4 6	0	8 4 5	1	12270.1229	0.0137

				Frequency	error
9 4 6	1	8 4 5	0	12271.0523	-0.0083
9 4 5	0	8 4 4	1	12302.9309	0.0112
9 4 5	1	8 4 4	0	12303.8959	0.0248
9 1 8	0	8 1 7	1	12305.0262	-0.0023
9 1 8	1	8 1 7	0	12305.9662	-0.0137
14 4 11	0	14 3 12	0	12337.6450	-0.0052
9 3 6	0	8 3 5	1	12583.3201	-0.0233
9 3 6	1	8 3 5	0	12584.2743	-0.0205
14 3 12	0	14 2 13	0	12684.2447	-0.0198
9 2 7	0	8 2 6	1	12900.1384	-0.0215
9 2 7	1	8 2 6	0	12901.1035	-0.0078
5 2 3	0	4 1 4	0	13004.2952	0.0224
8 2 7	0	7 1 6	0	13015.1948	-0.0058
13 1 12	0	13 0 13	0	13031.8545	0.0013
10 2 9	0	9 2 8	1	13067.2021	0.0035
10 2 9	1	9 2 8	0	13068.1560	0.0060
11 0 11	0	10 1 10	0	13249.1041	-0.0046
13 5 8	0	13 4 9	0	13295.7963	-0.0105
11 0 11	0	10 0 10	1	13308.6295	0.0024
11 0 11	1	10 0 10	0	13309.5721	-0.0062
4 3 2	0	3 2 1	0	13313.1941	-0.0015
13 2 12	0	13 1 13	0	13325.0406	0.0040
11 1 11	0	10 0 10	0	13343.8892	-0.0082
4 3 1	0	3 2 2	0	13403.5208	-0.0037
10 1 9	0	9 1 8	1	13476.8260	-0.0064
10 1 9	1	9 1 8	0	13477.7517	-0.0320
11 1 10	0	10 2 9	0	13570.3383	-0.0118
10 3 8	0	9 3 7	1	13570.7236	0.0146
10 3 8	1	9 3 7	0	13571.6652	0.0049
10 4 7	0	9 4 6	1	13655.9764	-0.0115
10 4 7	1	9 4 6	0	13656.9319	-0.0075

				Frequency	error
10 4 6	0	9 4 5	1	13724.6941	-0.0044
10 4 6	1	9 4 5	0	13725.6463	-0.0036
9 2 8	0	8 1 7	0	13759.6273	-0.0020
11 5 6	0	11 4 7	0	13878.9709	-0.0107
10 5 5	0	10 4 6	0	14043.1228	0.0268
13 5 9	0	13 4 10	0	14076.5639	-0.0203
12 5 8	0	12 4 9	0	14086.4079	-0.0202
14 5 10	0	14 4 11	0	14103.8719	-0.0010
10 3 7	0	9 3 6	1	14108.1530	-0.0277
10 3 7	1	9 3 6	0	14109.1367	0.0046
11 5 7	0	11 4 8	0	14118.4389	-0.0183
9 5 4	0	9 4 5	0	14151.0642	0.0279
9 5 5	0	9 4 6	0	14203.1541	-0.0109
8 5 3	0	8 4 4	0	14220.5227	0.0213
8 5 4	0	8 4 5	0	14241.0994	-0.0074
7 5 2	0	7 4 3	0	14264.3873	-0.0014
7 5 3	0	7 4 4	0	14271.4100	0.0112
11 2 10	0	10 2 9	1	14287.7084	0.0008
6 5 1	0	6 4 2	0	14291.4774	-0.0179
6 5 2	0	6 4 3	0	14293.4355	-0.0006
10 2 8	0	9 2 7	1	14305.4108	-0.0164
10 2 8	1	9 2 7	0	14306.3765	-0.0021
5 5 0	0	5 4 1	0	14307.6442	0.0036
5 5 1	0	5 4 2	0	14308.0253	-0.0076
12 0 12	0	11 1 11	0	14425.3890	0.0126
12 1 12	0	11 1 11	1	14444.7508	-0.0391
12 1 12	1	11 1 11	0	14445.7155	-0.0258
12 0 12	0	11 0 11	1	14459.6609	-0.0345
12 0 12	1	11 0 11	0	14460.6375	-0.0093
12 1 12	0	11 0 11	0	14480.0597	-0.0007
10 2 9	0	9 1 8	0	14521.8072	0.0078

				Frequency	error
5 3 3	0	4 2 2	0	14560.4310	-0.0021
11 1 10	0	10 1 9	1	14614.3694	0.0037
11 1 10	1	10 1 9	0	14615.2906	-0.0264
5 3 2	0	4 2 3	0	14831.9746	0.0042
11 3 9	0	10 3 8	1	14895.1380	0.0070
11 3 9	1	10 3 8	0	14896.0895	0.0072
11 5 7	0	10 5 6	1	15000.4340	0.0228
11 5 7	1	10 5 6	0	15001.3843	0.0217
5 3 2	0	5 0 5	0	15008.8878	0.0015
11 5 6	0	10 5 5	1	15009.1559	0.0155
11 5 6	1	10 5 5	0	15010.1151	0.0233
12 1 11	0	11 2 10	0	15018.1031	-0.0041
11 4 8	0	10 4 7	1	15042.3067	-0.0260
11 4 8	1	10 4 7	0	15043.3085	0.0243
6 2 4	0	5 1 5	0	15298.2335	0.0092
11 2 10	0	10 1 9	0	15332.6630	-0.0115
15 1 14	0	15 0 15	0	15431.3903	0.0095
12 2 11	1	11 2 10	0	15493.4575	0.0012
13 0 13	0	12 1 12	0	15593.5536	0.0037
13 1 13	0	12 1 12	1	15604.3103	0.0019
13 1 13	1	12 1 12	0	15605.2272	-0.0325
13 0 13	0	12 0 12	1	15612.9806	0.0172
13 0 13	1	12 0 12	0	15613.9249	0.0101
13 1 13	0	12 0 12	0	15624.6920	0.0188
11 3 8	0	10 3 7	1	15643.9752	-0.0287
11 2 9	0	10 2 8	1	15662.4772	-0.0122
11 2 9	1	10 2 8	0	15663.4499	0.0090
6 3 4	0	5 2 3	0	15709.8175	0.0024
12 1 11	0	11 1 10	1	15735.5014	0.0366
12 1 11	1	11 1 10	0	15736.4434	0.0273
12 2 11	0	11 1 10	0	16210.7824	-0.0313

				Frequency	error
6 3 3	0	5 2 4	0	16336.3206	-0.0038
4 4 1	0	3 3 0	0	16544.9905	-0.0104
4 4 0	0	3 3 1	0	16545.9890	-0.0028
7 3 5	0	6 2 4	0	16737.1312	-0.0014
14 0 14	0	13 1 13	0	16756.8775	-0.0078
14 1 14	0	13 1 13	1	16762.7091	0.0169
14 1 14	1	13 1 13	0	16763.6485	0.0050
14 1 14	0	13 0 13	0	16774.4019	-0.0001
13 1 12	0	12 1 11	1	16854.4699	0.0176
13 1 12	1	12 1 11	0	16855.4069	0.0032

				Frequency	error
12 2 10	0	11 2 9	1	16964.0319	-0.0086
12 2 10	1	11 2 9	0	16965.0017	0.0097
13 2 12	0	12 1 11	0	17159.3159	-0.0296
8 3 6	0	7 2 5	0	17634.6909	0.0002
7 2 5	0	6 1 6	0	17878.2032	-0.0195
5 4 2	0	4 3 1	0	17892.5951	0.0266
5 4 1	0	4 3 2	0	17899.5697	0.0075
15 0 15	0	14 1 14	0	17917.4138	0.0205
15 1 15	0	14 0 14	0	17927.1506	-0.0086
7 3 4	0	6 2 5	0	17958.0054	-0.0026

Table S15: Line list of transitions fitted for methyl guaiacol (**MG**).

			Frequency	error
5 2 4	5 1 5	A	6415.3299	0.0385
4 0 4	3 1 3	A	6415.7082	0.0044
2 2 1	1 1 0	A	6427.3997	0.0314
4 1 3	3 2 2	A	6428.7486	-0.0087
5 4 2	5 3 3	A	6531.4614	0.0403
6 3 4	6 2 5	A	6594.4191	0.0347
4 1 4	3 0 3	E	6690.2902	0.8962
4 1 4	3 0 3	A	6694.3409	0.0197
7 2 5	7 1 6	A	6703.4357	0.0134
6 4 3	6 3 4	A	6752.3171	0.0239
8 5 3	8 4 4	A	6788.6086	0.0476
3 3 1	2 2 0	E	6899.9862	-0.0812
2 2 0	1 1 1	A	7014.7139	0.0454
5 2 3	4 3 2	A	7029.6563	-0.0036
9 3 6	9 2 7	A	7362.0147	-0.0346
7 5 2	7 4 3	A	7499.4579	0.0207
7 3 5	7 2 6	A	7667.3132	0.0374
6 2 5	6 1 6	A	7728.2564	0.0615
3 2 2	2 1 1	A	7885.8571	0.041
8 4 5	8 3 6	A	7909.9257	0.0101
5 0 5	4 1 4	A	7962.3547	0.0039
6 5 1	6 4 2	A	7966.1642	0.0083
5 0 5	4 1 4	E	7968.6853	0.2005
5 1 5	4 0 4	E	8064.0664	0.4261
5 1 5	4 0 4	A	8065.7198	0.0173
5 5 1	5 4 2	A	8254.2384	0.0108
8 5 4	8 4 5	A	8298.2169	0.0124
10 6 4	10 5 5	A	8389.2905	0.0556
8 2 6	8 1 7	A	8430.1731	0.0108
5 1 4	4 2 3	A	8618.2348	0.0066

			Frequency	error
9 5 5	9 4 6	A	8621.6929	0.0162
4 2 3	3 1 2	E	8623.9468	2.2321
2 2 0	1 1 1	E	8793.2011	1.5436
9 4 6	9 3 7	A	8875.6232	0.0156
8 3 6	8 2 7	A	8914.6116	0.0391
7 1 6	7 0 7	A	9023.6266	0.0597
5 2 3	4 3 2	E	9099.998	-2.2733
7 2 6	7 1 7	A	9115.4776	0.0593
4 2 3	3 1 2	A	9120.1434	0.0415
10 5 6	10 4 7	A	9204.983	-0.0029
10 3 7	10 2 8	A	9212.5038	-0.0621
8 4 4	7 5 3	A	9327.9291	-0.0703
6 0 6	5 1 5	A	9453.6588	0.0233
6 0 6	5 1 5	E	9454.4391	0.3111
6 1 6	5 0 5	E	9486.6061	0.2135
6 1 6	5 0 5	A	9488.3448	0.0172
8 6 2	8 5 3	A	9662.2374	-0.0108
6 2 4	5 3 3	A	9779.1918	-0.0123
10 6 5	10 5 6	A	9828.6446	-0.0095
12 4 8	12 3 9	A	9850.4611	-0.1776
3 2 1	2 1 2	A	9858.6475	0.0508
7 3 4	6 4 3	A	9875.4143	-0.0532
8 6 3	8 5 4	A	9883.7893	-0.0165
7 6 1	7 5 2	A	9936.5584	-0.0282
10 4 7	10 3 8	A	10050.9247	-0.0014
11 5 7	11 4 8	A	10059.3915	-0.0353
9 2 7	9 1 8	A	10060.7496	0.0147
5 2 4	4 1 3	E	10074.2138	1.7391
6 6 0	6 5 1	A	10082.2189	-0.0219
6 6 1	6 5 2	A	10092.6661	-0.0228

			Frequency	error
5 2 4	4 1 3	A	10216.681	0.0537
9 3 7	9 2 8	A	10271.8125	0.0458
14 5 9	14 4 10	A	10358.714	-0.3294
3 3 1	2 2 0	A	10379.7247	0.0566
8 1 7	8 0 8	A	10504.3144	0.0348
6 1 5	5 2 4	A	10532.1363	0.0109
8 2 7	8 1 8	A	10537.3595	0.0635
3 3 0	2 2 1	A	10559.8363	0.0649
7 0 7	6 1 6	E	10921.7416	0.4359
7 0 7	6 1 6	A	10923.0387	0.0057
7 1 7	6 0 6	E	10931.886	-0.0361
7 1 7	6 0 6	A	10933.9767	0.0083
6 2 4	5 3 3	E	10964.8748	-0.9364
11 3 8	11 2 9	A	10971.6321	-0.0792
3 2 1	2 1 2	E	11214.4479	0.6308
6 2 5	5 1 4	E	11296.4229	0.5266
6 2 5	5 1 4	A	11325.6003	0.0262
11 4 8	11 3 9	A	11371.2856	-0.0134
11 7 5	11 6 6	A	11414.7867	-0.0576
10 7 4	10 6 5	A	11553.9976	-0.0559
10 2 8	10 1 9	A	11603.2806	-0.0011
9 7 2	9 6 3	A	11650.5331	-0.0696
10 3 8	10 2 9	A	11686.6159	0.0159
9 7 3	9 6 4	A	11708.6671	-0.0795
8 7 1	8 6 2	A	11829.6678	-0.0824
8 7 2	8 6 3	A	11842.3778	-0.0836
7 7 0	7 6 1	A	11940.7545	-0.0999
7 7 1	7 6 2	A	11942.683	-0.1044
9 1 8	9 0 9	A	11961.4579	0.0525
9 2 8	9 1 9	A	11972.6459	0.055
4 3 2	3 2 1	A	11994.264	0.0628

			Frequency	error
7 1 6	6 2 5	A	12218.4136	0.0087
14 6 9	14 5 10	A	12235.7928	-0.1785
7 1 6	6 2 5	E	12241.1307	0.4264
7 2 5	6 3 4	A	12327.4107	-0.0321
8 0 8	7 1 7	E	12382.5906	0.8585
8 0 8	7 1 7	A	12384.7787	0.0041
8 1 8	7 0 7	E	12385.6462	-0.5492
8 1 8	7 0 7	A	12388.0866	0.0093
13 5 9	13 4 10	A	12426.8744	-0.1178
7 2 6	6 1 5	E	12546.1134	-0.272
7 2 6	6 1 5	A	12555.6257	0.0203
9 4 5	8 5 4	A	12589.8819	-0.1095
12 3 9	12 2 10	A	12604.8152	-0.0958
12 4 9	12 3 10	A	12775.619	-0.0626
7 2 5	6 3 4	E	12841.3203	1.2091
4 3 1	3 2 2	A	12860.4568	0.0704
8 3 5	7 4 4	A	12960.2914	-0.0626
13 8 6	13 7 7	A	13018.4069	-0.1073
11 2 9	11 1 10	A	13095.4768	-0.043
11 3 9	11 2 10	A	13126.2298	-0.0122
6 3 4	5 2 3	E	13289.336	1.9302
5 3 3	4 2 2	A	13298.5317	0.0342
4 2 2	3 1 3	A	13351.2594	0.0826
10 1 9	10 0 10	A	13408.3854	0.0626
8 1 7	7 2 6	A	13773.6391	0.0032
8 1 7	7 2 6	E	13776.6815	0.1378
9 0 9	8 1 8	E	13841.4541	1.4233
9 1 9	8 0 8	E	13842.3458	-1.2036
9 0 9	8 1 8	A	13844.0826	0.0073
9 1 9	8 0 8	A	13845.0431	0.0008
8 2 7	7 1 6	E	13894.1279	-0.5729

			Frequency	error
8 2 7	7 1 6	A	13901.8291	0.0226
13 3 10	13 2 11	A	14152.3938	-0.0936
4 4 1	3 3 0	A	14249.1422	0.1103
4 4 0	3 3 1	A	14288.0424	0.0584
6 3 4	5 2 3	A	14338.4079	0.0459
8 2 6	7 3 5	A	14536.4581	-0.0645
12 2 10	12 1 11	A	14563.1969	-0.0381
12 3 10	12 2 11	A	14573.9645	-0.0428
8 2 6	7 3 5	E	14720.6248	2.4219
11 1 10	11 0 11	A	14850.779	0.0022
11 2 10	11 1 11	A	14851.9576	0.0424
7 3 5	6 2 4	A	15222.8589	0.0331
9 1 8	8 2 7	E	15263.7994	-0.2278
9 1 8	8 2 7	A	15268.1779	-0.0068
10 0 10	9 1 9	E	15299.7768	1.8005
10 1 10	9 0 9	E	15300.0395	-1.7301
10 0 10	9 1 9	A	15302.6578	-0.0065
10 1 10	9 0 9	A	15302.9318	-0.0089
9 2 8	8 1 7	E	15305.3124	-0.7673
9 2 8	8 1 7	A	15313.36	0.0064
5 3 2	4 2 3	A	15657.8164	0.0433
14 4 11	14 3 12	A	15679.0271	-0.1462
7 4 4	6 3 3	E	15693.9538	2.5653
9 3 6	8 4 5	A	15866.3751	-0.1058
10 4 6	9 5 5	A	15970.1638	-0.1947
8 3 6	7 2 5	E	16014.2418	-2.6632

			Frequency	error
13 2 11	13 1 12	A	16019.1622	-0.0997
13 3 11	13 2 12	A	16022.7979	-0.0966
5 4 2	4 3 1	A	16069.4549	0.059
8 3 6	7 2 5	A	16113.0056	0.0489
12 1 11	12 0 12	A	16291.1229	0.0322
12 2 11	12 1 12	A	16291.4659	0.0274
5 4 1	4 3 2	A	16335.02	0.0795
9 2 7	8 3 6	A	16414.2907	-0.0564
9 2 7	8 3 6	E	16472.7046	1.6268
10 1 9	9 2 8	E	16730.8305	-0.4595
10 1 9	9 2 8	A	16738.4297	0.0336
10 2 9	9 1 8	E	16744.771	-1.1128
10 2 9	9 1 8	A	16753.5114	0.0247
11 0 11	10 1 10	E	16757.9609	1.9579
11 1 11	10 0 10	E	16758.0788	-2.1357
11 0 11	10 1 10	A	16761.0125	-0.059
11 1 11	10 0 10	A	16761.185	0.036
9 3 7	8 2 6	E	17127.083	-3.7804
15 3 12	15 2 13	A	17131.6023	-0.2404
9 3 7	8 2 6	A	17154.9594	0.0015
5 2 3	4 1 4	A	17434.9785	0.083
6 4 3	5 3 2	A	17632.7752	0.0683
13 1 12	13 0 13	A	17730.1968	-0.0263
13 2 12	13 1 13	A	17730.4039	0.0767
8 5 4	7 4 3	E	17759.8378	-1.8049

Table S16: Line list of transitions fitted for vinyl guaiacol (***Z*-VG**).

		Frequency	error
3 2 1	2 1 2	8099.3394	0.0040
7 0 7	6 1 6	8178.5230	0.0245
4 2 3	3 1 2	8250.2626	-0.0168
7 1 7	6 0 6	8402.4466	-0.0034
5 2 4	4 1 3	9130.8599	-0.0064
8 1 8	7 0 7	9453.8389	-0.0140
8 1 7	7 2 6	9559.5724	-0.0068
6 2 5	5 1 4	9924.6282	-0.0010
3 3 1	2 2 0	9992.0935	-0.0030
3 3 0	2 2 1	10026.9579	0.0000
4 2 2	3 1 3	10054.4036	0.0282
9 0 9	8 1 8	10469.9039	-0.0161
9 1 9	8 0 8	10529.4340	-0.0154
9 1 8	8 2 7	11023.3616	-0.0025
4 3 2	3 2 1	11257.1394	-0.0126
8 2 7	7 1 6	11413.3581	0.0048
4 3 1	3 2 2	11432.9465	0.0105
10 0 10	9 1 9	11589.7834	0.0071
10 1 10	9 0 9	11619.1907	-0.0048
9 2 8	8 1 7	12207.5334	0.0098
5 2 3	4 1 4	12333.8162	0.0206
10 1 9	9 2 8	12368.9614	-0.0132
5 3 3	4 2 2	12410.5151	-0.0095
11 0 11	10 1 10	12702.3982	0.0143
11 1 11	10 0 10	12716.6423	0.0028
5 3 2	4 2 3	12931.4785	-0.0014
6 3 4	5 2 3	13415.3305	0.0060
11 1 10	10 2 9	13623.1699	0.0177
4 4 1	3 3 0	13744.2911	-0.0065
4 4 0	3 3 1	13747.3575	-0.0031
12 0 12	11 1 11	13811.2984	0.0081
12 1 12	11 0 11	13818.0878	-0.0026
7 3 5	6 2 4	14264.9917	0.0271
6 3 3	5 2 4	14588.1297	0.0103
12 1 11	11 2 10	14815.1616	-0.0060
13 0 13	12 1 12	14918.3700	0.0030
13 1 13	12 0 12	14921.5595	-0.0097
6 2 4	5 1 5	14953.8886	-0.0064
8 3 6	7 2 5	14977.5401	-0.0031
5 4 2	4 3 1	15074.8113	0.0029
5 4 1	4 3 2	15096.4345	0.0060
6 4 3	5 3 2	16373.2892	-0.0137
6 4 2	5 3 3	16459.7438	0.0063
7 3 4	6 2 5	16481.9604	-0.0196
7 4 3	6 3 4	17858.8707	-0.0116

Table S17: Line list of transitions fitted for vinyl guaiacol (***E*-VG**).

		Frequency	error
10 4 7	10 3 8	8043.4980	-0.0252
8 5 4	8 4 5	8060.4431	-0.0037
6 5 1	6 4 2	8067.1978	-0.0088
7 5 3	7 4 4	8078.7874	0.0091
9 5 5	9 4 6	8109.9810	-0.0202
6 5 2	6 4 3	8124.7141	-0.0034
8 2 7	8 1 8	8231.0860	0.0441
7 2 5	6 3 4	8282.4073	-0.0206
5 2 4	4 1 3	8517.5910	-0.0007
7 0 7	6 1 6	8570.2243	-0.0070
7 1 7	6 0 6	8610.7466	-0.0056
10 2 8	10 1 9	8657.2011	0.0054
11 4 8	11 3 9	8857.8910	-0.0373
3 3 1	2 2 0	8925.3840	0.0008
3 3 0	2 2 1	9007.8715	-0.0019
10 3 8	10 2 9	9032.6079	-0.0099
7 1 6	6 2 5	9317.4030	0.0043
6 2 5	5 1 4	9329.0765	-0.0057
9 2 8	9 1 9	9345.8653	0.0183
10 6 4	10 5 5	9362.9817	-0.0119
10 6 5	10 5 6	9709.4718	0.0095
8 0 8	7 1 7	9727.5974	-0.0017
8 1 8	7 0 7	9743.3891	-0.0007
9 6 4	9 5 5	9787.3114	0.0076
8 6 2	8 5 3	9830.1474	0.0156
7 6 1	7 5 2	9931.7137	0.0041
7 6 2	7 5 3	9941.6394	-0.0048
11 3 9	11 2 10	10121.5487	0.0085
7 2 6	6 1 5	10172.9068	0.0039
4 3 2	3 2 1	10224.0670	0.0088
4 2 2	3 1 3	10323.7800	0.0007
8 2 6	7 3 5	10324.8709	-0.0018
4 3 1	3 2 2	10632.6333	0.0124
8 1 7	7 2 6	10678.2246	0.0054
9 0 9	8 1 8	10877.8183	-0.0029
9 1 9	8 0 8	10883.7787	-0.0036
8 2 7	7 1 6	11107.1209	-0.0038
5 3 3	4 2 2	11325.5037	0.0041
9 1 8	8 2 7	11933.6565	0.0168
10 0 10	9 1 9	12025.2000	0.0127
10 1 10	9 0 9	12027.3842	0.0000
9 2 8	8 1 7	12131.5949	-0.0061
9 2 7	8 3 6	12169.9305	0.0025
6 3 4	5 2 3	12223.0247	-0.0025
4 4 1	3 3 0	12254.8637	-0.0275
4 4 0	3 3 1	12267.3131	-0.0075
10 3 7	9 4 6	12445.1961	-0.0075
5 3 2	4 2 3	12490.1107	-0.0044
7 3 5	6 2 4	12956.3940	-0.0112
10 1 9	9 2 8	13130.2423	-0.0054
11 0 11	10 1 10	13171.4762	0.0021
11 1 11	10 0 10	13172.2683	-0.0003
10 2 9	9 1 8	13216.3361	-0.0072
8 3 6	7 2 5	13592.7398	0.0149
5 4 2	4 3 1	13678.9507	0.0032
5 4 1	4 3 2	13765.8193	0.0040
10 2 8	9 3 7	13783.4924	0.0034
9 3 7	8 2 6	14223.7822	-0.0112
11 1 10	10 2 9	14297.6978	0.0006
12 0 12	11 1 11	14317.3856	0.0087

		Frequency	error
12 1 12	11 0 11	14317.6686	0.0087
6 3 3	5 2 4	14715.1155	-0.0005
10 3 8	9 2 7	14943.1378	0.0281
6 4 3	5 3 2	14997.4577	0.0036
11 2 9	10 3 8	15201.5427	0.0152
6 4 2	5 3 3	15334.0517	-0.0106
13 0 13	12 1 12	15463.1335	-0.0209
13 1 13	12 0 12	15463.2875	0.0335
12 2 11	11 1 10	15466.2913	-0.0388
5 5 1	4 4 0	15554.3461	0.0060
5 5 0	4 4 1	15555.9229	0.0183
11 3 9	10 2 8	15797.8888	-0.0032

		Frequency	error
6 2 4	5 1 5	16462.9798	0.0024
12 2 10	11 3 9	16488.9628	0.0386
13 1 12	12 2 11	16600.4632	-0.0139
14 0 14	13 1 13	16608.9239	0.0254
14 1 14	13 0 13	16608.9239	-0.0092
12 3 10	11 2 9	16774.1338	-0.0111
6 5 2	5 4 1	17013.5820	0.0035
6 5 1	5 4 2	17027.6518	-0.0141
7 4 3	6 3 4	17060.6906	-0.0098
15 0 15	14 1 14	17754.6274	-0.0112
15 1 15	14 0 14	17754.6274	-0.0232