Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

The Interplay of Hydrogen Bonding and Dispersion in Phenol Dimer and Trimer: Structures from Broadband Rotational Spectroscopy

SUPPORTING INFORMATION

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Figure S1. Schematic structure of phenol dimer, with the numbering used in this supplement.

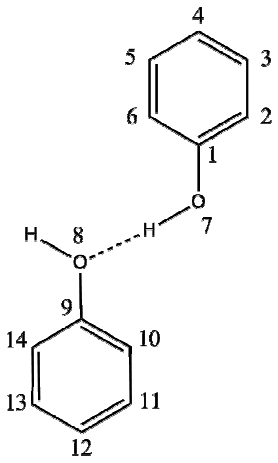

Table S1. *Ab initio* spectroscopic and select structural parameters for phenol dimer, between experiment (from this study and Ref. 24) and multiple levels of theory.

	MP2/6-311g(d,p)	MP2/6-311++g(d,p)	MP2/cc-PVTZ-cp
A	1165.1709	1365.1581	1285.9792
B	410.2755	325.7977	356.14872
C	363.2810	305.6706	317.56969
Hinge Angle	49.0	69.5	48.2
r(O … O)	2.84	2.88	2.89
t(C10-C9-O8-H7)	34.3	14.0	29.2
μ_a / D	2.7	2.8	2.9
μ_b / D	-0.63	-0.48	-0.40
μ_c / D	1.8	1.9	1.5

	M062X/6-311g(d,p)	M062X/6-311++g(d,p)	M062X/6-311++g(df,pd)
A	1352.7189	1382.5289	1382.8902
B	342.0526	336.5921	338.42239
C	318.2536	306.4143	307.56143
Hinge Angle	68.2	59.6	59.6
r(O … O)	2.85	2.84	2.84
t(C10-C9-O8-H7)	11.9	13.5	11.5
μ_a / D	2.9	3.1	3.1
μ_b / D	-0.26	-0.38	-0.33
μ_c / D	1.9	1.7	1.7

	B3LYP/6-31G(d,p)	B3LYP/6-311++g(d,p)	RI-DFT-D/aQz'
A	1799.9670	1946.2522	1399.7
B	250.8155	231.8222	318.5
C	243.6506	229.5711	292.5
Hinge Angle	111.9	110.5	61
r(O … O)	2.86	2.88	--
t(C10-C9-O8-H7)	-4.6	-25.0	--
ua	-2.8	3.1	--
ub	-2.1	0.21	--
uc	0.085	1.7	--

	Experiment (r_0)	Schmitt et al
μ_a / D	1415.32747(14)	1416.99(39)
μ_b / D	313.368020(41)	313.51(1)
μ_c / D	287.961282(38)	288.11(1)
Hinge Angle	62.3(14)	63 (rs)
r(O … O)	2.8326(211)	3.21
t(C10-C9-O8-H7)	10.6(17)	-1.8(22)
μ_a / D	3 (relative)	--
μ_b / D	0.5 (relative)	--
μ_c / D	2 (relative)	--

Table S2. Coordinates for the heavy atoms of the M06-2X/6-311++g(d,p) theoretical structure for phenol dimer, with center of mass distances. All values are in Angstroms.

	a	b	c	COM Dist
Donor				
1-	-2.036241	0.738326	-0.183119	2.17369
ortho (2-)	-1.548847	-0.120365	0.802707	1.74864
meta (3-)	-2.288539	-1.241304	1.167227	2.85319
para (4-)	-3.509243	-1.514053	0.560968	3.86288
meta (5-)	-3.988752	-0.649666	-0.420948	4.06318
ortho (6-)	-3.260639	0.470832	-0.795057	3.38904
O	-1.360876	1.842696	-0.591067	2.36577
Acceptor				
1-	2.033176	0.72657	0.183237	2.16686
ortho (2-)	3.238263	0.465605	0.823726	3.37367
meta (3-)	3.986402	-0.643743	0.442742	4.06224
para (4-)	3.531735	-1.485748	-0.565015	3.87296
meta (5-)	2.32049	-1.21108	-1.194531	2.87720
ortho (6-)	1.563603	-0.10621	-0.826591	1.77183
O	1.252137	1.805041	0.525676	2.25884

Table S3. Coordinates for the heavy atoms of the MP2/6-311++g(d,p) theoretical structure for phenol dimer, with center of mass distances. All values are in Angstroms.

	a	b	c	COM Dist
Donor				
1-	-2.022736	0.703599	-0.225572	2.15346
ortho (2-)	-1.617708	-0.09508	0.850205	1.82999
meta (3-)	-2.421426	-1.161893	1.257553	2.96559
para (4-)	-3.616977	-1.445464	0.596136	3.94047
meta (5-)	-4.011513	-0.643483	-0.478824	4.09091
ortho (6-)	-3.219565	0.425182	-0.893882	3.36829
O	-1.284589	1.764754	-0.684735	2.28766
Acceptor				
1-	2.058278	0.707128	0.251387	2.19083
ortho (2-)	3.215449	0.346157	0.940383	3.36798
meta (3-)	3.970240	-0.736533	0.482906	4.06675
para (4-)	3.565769	-1.452488	-0.644142	3.90376
meta (5-)	2.40172	-1.076205	-1.320623	2.94457
ortho (6-)	1.637497	0.001686	-0.877397	1.85775
O	1.263548	1.771264	0.654168	2.27197

Table S4. Coordinates for the r_s (Kraitchman) experimental structure of phenol dimer, with center of mass distances. All values are in Angstroms.

	a	b	c	COM Dist
Donor				
1-	2.10773(73)	0.7094(22)	0.1689(91)	2.2303(21)
ortho (2-)	1.60536(99)	0.2655(60)	0.76519(21)	1.7981(26)
meta (3-)	2.41212(71)	1.3028(13)	1.1143(15)	2.9593(17)
para (4-)	3.69224(44)	1.4774(11)	0.5428(30)	4.1955(12)
meta (5-)	4.13547(39)	0.5636(29)	0.4269(38)	4.1956(51)
ortho (6-)	3.35229(48)	0.5146(31)	0.7885(21)	3.4820(14)
O7	1.3382(14)	1.8048(10)	0.6006(32)	2.3257(24)
Acceptor				
1-	2.08195(79)	0.7341(22)	0.1652(99)	2.2138(22)
ortho (2-)	3.30550(47)	0.4666(33)	0.8617(18)	3.4478(61)
meta (3-)	4.09836(39)	0.6065(26)	0.4732(34)	4.1699(11)
para (4-)	3.67466(42)	1.4911(10)	0.5120(30)	3.9986(12)
meta (5-)	2.46944(64)	1.2047(13)	1.2118(13)	3.0030(16)
ortho (6-)	1.61137(97)	0.2675(59)	0.8427(19)	1.8380(26)
O8	1.2001(18)	1.7727(12)	0.5340(41)	2.2064(29)

Table S5. Coordinates for the r_0 experimental structure of phenol dimer, using the M06-2X/6-311++g(d,p) geometry as the reference geometry. All values are in Angstroms.

	a	b	c
Donor			
1-	-2.0992(35)	0.7053(39)	-0.1928(75)
ortho (2-)	-1.6528(74)	-0.193(12)	0.777(12)
meta (3-)	-2.4555(87)	-1.271(12)	1.140(11)
para (4-)	-3.6981(63)	-1.4591(75)	0.547(11)
meta (5-)	-4.1350(68)	-0.5556(92)	-0.419(12)
ortho (6-)	-3.3432(64)	0.5218(70)	-0.7907(92)
O	-1.340(13)	1.804(11)	-0.610(16)
Acceptor			
1-	2.1289(68)	0.725(11)	0.1997(68)
ortho (2-)	3.3083(76)	0.528(22)	0.907(15)
meta (3-)	4.1290(86)	-0.581(18)	0.426(15)
para (4-)	3.6934(76)	-1.4627(70)	-0.5558(107)
meta (5-)	2.4620(94)	-1.253(22)	-1.170(13)
ortho (6-)	1.6656(101)	-0.173(24)	-0.8136(107)
O	1.267(16)	1.764(11)	0.497(15)

Table S6. Full listing of structural parameters for two theoretical structures from phenol dimer, one from M06-2X/6-311++g(d,p) and the other from the benchmark MP2/cc-pVTZ-cp calculation taken from Ref 19.

Intramolecular Parameters	*M06-2X/6-311++g(d,p)*	MP2/cc-pVTZ-cp
Bond lengths (Å)		
Donor		
C1-C2	1.39499	1.39531
C2-C3	1.38772	1.39224
C3-C4	1.39284	1.38962
C4-C5	1.38962	1.39284
C5-C6	1.39224	1.38772
C6-C1	1.39531	1.39237
C1-O7	1.38745	1.36173
O7-H7	0.96844	0.96844
Acceptor		
C9-C10	1.39184	1.39156
C10-C11	1.38843	1.39342
C11-C12	1.39211	1.39213
C12-C13	1.38953	1.39410
C13-C14	1.39146	1.39107
C14-C9	1.38932	1.39235
C9-O8	1.37449	1.37783
O8-H8	0.96179	0.96335

Angles (°)	*M06-2X/6-311++g(d,p)*	MP2/cc-pVTZ-cp
Donor		
<(C1-C2-C3)	119.804	120.026
<(C2-C3-C4)	120.687	120.565
<(C3-C4-C5)	119.251	119.267
<(C4-C5-C6)	120.673	120.559
<(C5-C6-C1)	119.674	119.934
<(C6-C1-C2)	119.911	119.649
<(C6-C1-O7)	122.610	122.922
<(C2-C1-O7)	117.478	117.429
<(C1-O7-H7)	110.385	108.980
Acceptor		
<(C9-C10-C11)	118.979	119.547
<(C10-C11-C12)	120.745	120.282
<(C11-C12-C13)	119.578	119.570
<(C12-C13-C14)	120.369	120.460
<(C13-C14-C9)	119.329	119.237

<(C14-C9-C10)	121.000	120.723
<(C10-C9-O8)	117.232	117.22
<(C14-C9-O8)	121.765	122.054
<(C9-O8-H8)	110.607	108.555

Dihedrals (°)	*M06-2X/6-311++g(d,p)*	MP2/cc-pVTZ-cp
Donor		
t(C1-C2-C3-C4)	0	0
t(C2-C3-C4-C5)	0	0
t(C3-C4-C5-C6)	0	0
t(C4-C5-C6-C1)	0	0
t(C5-C6-C1-C2)	0	0
t(C6-C1-C2-C3)	0	0
t(C6-C1-O7-H7)	-178.424	-176.132
t(C2-C1-O7-H7)	1.244	3.744
Acceptor		
t(C9-C10-C11-C12)	0	0
t(C10-C11-C12-C13)	0	0
t(C11-C12-C13-C14)	0	0
t(C12-C13-C14-C9)	0	0
t(C13-C14-C9-C10)	0	0
t(C14-C9-C10-C11)	0	0
t(C14-C9-O8-H8)	-178.088	-177.829
t(C10-C9-O8-H8)	2.482	2.766

Intermolecular Parameters	*M06-2X/6-311++g(d,p)*	MP2/cc-pVTZ-cp
Bond lengths (Å)		
r(O7-O8)	2.84397	2.89043
r(H7-O8)	1.88945	1.93721
Angles (°)		
<(C1-O7-O8)	109.508	110.825
<(O7-O8-C9)	115.160	113.213
<(O7-H7-O8)	168.046	167.200
<(C9-O8-H7)	118.882	115.745
Dihedrals (°)		
t(C2-C1-O7-O8)	-170.689	-167.387
t(C1-O7-O8-C9)	59.607	48.173
t(O7-O8-C9-C10)	11.816	25.474
t(O8-H7-O7-C1)	85.073	103.967
t(C9-O8-H7-O7)	-23.415	-54.330
t(C10-C9-O8-H7)	13.590	29.240

Table S7. Full listing of structural parameters for three experimental structures from phenol dimer: 1) the Kraitchman r_s structure; 2) r_0 structure with the M06-2X/6-311++g(d,p) reference geometry; 3) r_0 structure with benchmark MP2/cc-pVTZ-cp reference geometry, taken from Ref 19. Values from the r_0 fit from Schmitt et al.[24] are added for comparison. In the case of intramolecular parameters from Schmitt et al., the direct reporting of which are omitted, the values assumed by the authors are taken from a previous microwave study on phenol monomer.[§]

Intramolecular Parameters	r_s, this work	r_0, MP2	r_0, M06-2X	r_0, Schmitt et al.
Bond lengths (Å)				
Donor				
C1-C2	1.4319(45)	1.396(15)	1.3924(84)	1.3912(46)
C2-C3	1.3809(35)	1.391(19)	1.3877(112)	1.3944(50)
C3-C4	1.3849(39)	1.394(24)	1.3928(140)	1.3954(36)
C4-C5	1.4148(17)	1.393(20)	1.3896(119)	1.3954(36)
C5-C6	1.3522(44)	1.393(25)	1.3922(153)	1.3922(50)
C6-C1	1.4464(79)	1.396(22)	1.3953(130)	1.3912(46)
C1-O7	1.4113(61)	1.354(42)	1.3987(132)	1.3745(45)
O7-H7	--	0.969(37)	0.9684(220)	0.9574(57)
Acceptor				
C9-C10	1.4913(75)	1.407(33)	1.4310(192)	1.3912(46)
C10-C11	1.3367(47)	1.391(48)	1.3884(268)	1.3944(50)
C11-C12	1.4115(16)	1.394(24)	1.3921(135)	1.3954(36)
C12-C13	1.3902(37)	1.392(31)	1.3895(183)	1.3954(36)
C13-C14	1.3896(34)	1.549(82)	1.4613(236)	1.3922(50)
C14-C9	1.4049(47)	1.391(23)	1.3893(125)	1.3912(46)
C9-O8 *	1.388(14)	1.351(38)	1.3819(166)	1.3745(45)
O8-H8	--	0.963(40)	0.9618(228)	0.9574(57)

Angles (°)	r_s, this work	r_0, MP2	r_0, M06-2X	r_0, Schmitt et al.
Donor				
<(C1-C2-C3)	120.59(31)	120.0(12)	119.80(73)	119.43(31)
<(C2-C3-C4)	120.01(14)	120.6(12)	120.69(72)	120.48(26)
<(C3-C4-C5)	119.88(12)	119.3(13)	119.25(78)	119.24(22)
<(C4-C5-C6)	121.01(15)	120.6(17)	120.61(98)	120.79(26)
<(C5-C6-C1)	118.82(10)	119.9(13)	119.67(75)	119.22(31)
<(C6-C1-C2)	117.79(26)	119.65(95)	119.97(57)	120.85(36)
<(C6-C1-O7)	118.09(44)	122.9(14)	122.61(77)	122.14(31)
<(C2-C1-O7)	123.59(66)	117.4(14)	117.42(79)	117.01(33)

[§] Larsen, N.W. *J. Mol. Struct.* **1979**, *51*, 175-190.

<(C1-O7-H7)	--	109.0(25)	110.4(15)	108.77(35)
Acceptor				
<(C9-C10-C11)	116.47(12)	119.2(17)	118.98(97)	119.43(31)
<(C10-C11-C12)	123.54(16)	120.6(23)	120.7(13)	120.48(26)
<(C11-C12-C13)	119.35(12)	119.6(19)	119.6(11)	119.24(22)
<(C12-C13-C14)	121.04(13)	122.0(15)	122.54(92)	120.79(26)
<(C13-C14-C9)	118.82(30)	109.7(21)	114.7(14)	119.22(31)
<(C14-C9-C10)	120.34(25)	125.8(24)	123.1(13)	120.85(36)
<(C10-C9-O8)	117.16(69)	115.93(18)	114.99(90)	117.01(33)
<(C14-C9-O8)	122.07(81)	122.0(21)	121.8(12)	122.14(31)
<(C9-O8-H8)	--	103.9(29)	106.2(17)	108.77(35)

Dihedrals (°)	r_s, this work	r_0, MP2	r_0, M06-2X	r_0, Schmitt et al.
Donor				
t(C1-C2-C3-C4)	-0.25(50)	[0]	[0]	"
t(C2-C3-C4-C5)	3.34(38)	[0]	[0]	"
t(C3-C4-C5-C6)	-12.02(34)	[0]	[0]	"
t(C4-C5-C6-C1)	16.84(53)	[0]	[0]	"
t(C5-C6-C1-C2)	-13.26(76)	[0]	[0]	"
t(C6-C1-C2-C3)	5.03(73)	[0]	[0]	"
t(C6-C1-O7-H7)	--	[-176.132]	[-178.424]	"
t(C2-C1-O7-H7)	--	[3.744]	[1.244]	"
Acceptor				
t(C9-C10-C11-C12)	-0.78(46)	[0]	[0]	"
t(C10-C11-C12-C13)	3.71(34)	[0]	[0]	"
t(C11-C12-C13-C14)	-0.75(36)	[0]	[0]	"
t(C12-C13-C14-C9)	-4.95(45)	[0]	[0]	"
t(C13-C14-C9-C10)	7.87(65)	[0]	[0]	"
t(C14-C9-C10-C11)	-5.06(67)	[0]	[0]	"
t(C14-C9-O8-H8)	--	[-177.829]	[-178.008]	"
t(C10-C9-O8-H8)	--	[2.766]	[2.482]	"

Intermolecular Parameters	r_s, this work	r_0, MP2	r_0, M06-2X	r_0, Schmitt et al.
Bond lengths (Å)				
r(O7-O8)	2.7808(173)	2.830(36)	2.8326(211)	3.21
r(H7-O8)	--	1.879(38)	1.8730(226)	2.354(49)
Angles (°)				
<(C1-O7-O8)	118.24(58)	114.5(24)	111.84(79)	112.7
<(O7-O8-C9)	118.05(80)	120.4(15)	120.02(86)	117.1
<(O7-H7-O8)	--	166.2(37)	170.5(21)	150.6(18)
<(C9-O8-H7)	--	125.8(28)	122.5(10)	138.6(15)
Dihedrals (°)				
t(C2-C1-O7-O8)	-170.64(54)	-168.3(23)	-172.52(62)	-174.3
t(C1-O7-O8-C9)	64.0(13)	56.5(37)	62.3(14)	63.0
t(O7-O8-C9-C10)	5.9(11)	14.5(36)	8.1(14)	12.2
t(O8-H7-O7-C1)	--	87(12)	75.5(59)	80.6(47)
t(C9-O8-H7-O7)	--	-35(10)	-27.7(47)	-26.5(46)
t(C10-C9-O8-H7)	--	14.8(44)	10.6(17)	-1.0(19)

Table S8. Coordinates for the M06-2X/6-311++g(d,p) geometry of phenol dimer

C	-2.02924	0.737162	-0.17893
O	-1.35395	1.84384	-0.58089
H	-0.51248	1.915585	-0.10834
C	-1.53648	-0.13236	0.794647
C	-2.27599	-1.2547	1.15459
C	-3.50235	-1.51845	0.555911
C	-3.98713	-0.64354	-0.41394
C	-3.25908	0.478438	-0.78368
H	-0.57978	0.071336	1.263565
H	-1.88422	-1.9255	1.910426
H	-4.07408	-2.39275	0.840808
H	-4.94314	-0.83565	-0.88734
H	-3.62335	1.168573	-1.53483
O	1.263122	1.817416	0.531818
C	2.034191	0.732656	0.185545
H	1.686841	2.324769	1.229765
C	1.566243	-0.07869	-0.84252
C	2.311071	-1.18997	-1.21529
C	3.509346	-1.49149	-0.57337
C	3.962947	-0.67036	0.451986
C	3.22626	0.444916	0.838552
H	0.632467	0.16909	-1.33435
H	1.948741	-1.82534	-2.01455
H	4.083251	-2.36023	-0.87029
H	4.893786	-0.89416	0.959087
H	3.577876	1.086896	1.640355

Table S9. List of assigned transitions for phenol dimer, parent species

J'	K_a '	K_c '	←	J''	K_a''	K_c ''	ν_{obs} (MHz)	ν_{obs} - ν_{calc}
13	2	12	←	12	3	10	2100.5388	0.0021
14	2	13	←	14	1	13	2114.5220	0.0032
13	2	12	←	13	1	12	2264.0086	0.0031
13	1	12	←	13	1	13	2271.8368	0.0052
6	0	6	←	5	1	4	2275.3346	0.0016
4	1	4	←	3	1	3	2353.6079	0.0016
2	1	1	←	1	0	1	2355.4247	0.0008
8	4	4	←	9	3	6	2375.5821	-0.0002
11	1	11	←	10	2	9	2393.6834	-0.0172
4	0	4	←	3	0	3	2400.8914	0.0009
4	2	3	←	3	2	2	2405.0120	0.0017
4	3	2	←	3	3	1	2406.3692	0.0114
12	2	11	←	12	1	11	2407.4767	0.0019
4	2	2	←	3	2	1	2409.3423	0.0008
4	1	3	←	3	1	2	2455.1657	0.0007
9	1	8	←	8	2	6	2524.4185	0.0011
11	2	10	←	11	1	10	2543.6103	0.0014
4	3	1	←	5	2	3	2553.5479	-0.0094
4	3	2	←	5	2	4	2568.6711	0.0091
14	1	13	←	14	1	14	2606.9752	0.0016
13	2	11	←	12	3	9	2611.0027	-0.0003
17	3	14	←	16	4	12	2616.5136	0.0020
14	2	13	←	13	3	11	2655.2513	-0.0013
10	2	9	←	10	1	9	2671.2886	0.0008
7	0	7	←	6	1	5	2779.9958	0.0012
9	2	8	←	9	1	8	2789.5763	0.0005
12	1	12	←	11	2	10	2830.9810	0.0011
8	2	7	←	8	1	7	2897.7035	0.0006
5	1	5	←	4	1	4	2941.1711	0.0017
7	4	3	←	8	3	5	2981.4812	-0.0030
3	1	2	←	2	0	2	2995.0134	0.0047
5	0	5	←	4	0	4	2997.8242	0.0013
5	2	4	←	4	2	3	3005.6569	0.0024
5	4	1	←	4	4	0	3008.0513	0.0007
5	3	3	←	4	3	2	3008.2578	0.0017
5	3	2	←	4	3	1	3008.3572	0.0038
5	2	3	←	4	2	2	3014.2926	0.0013
18	3	16	←	17	4	14	3053.8325	0.0008
5	1	4	←	4	1	3	3068.0359	0.0012
6	2	5	←	6	1	5	3081.0970	-0.0007
5	2	4	←	5	1	4	3155.4692	0.0005
10	1	9	←	9	2	7	3190.8758	0.0007
15	2	14	←	14	3	12	3200.3810	-0.0011

4	2	3	←	4	1	3	3217.8485	-0.0004
13	1	13	←	12	2	11	3253.8582	0.0013
8	0	8	←	7	1	6	3262.7897	0.0009
3	2	2	←	3	1	2	3268.0027	-0.0009
18	3	15	←	17	4	13	3275.4641	0.0001
2	2	1	←	2	1	1	3305.7603	0.0011
14	2	12	←	13	3	10	3310.0227	-0.0032
2	2	0	←	2	1	2	3382.4012	0.0002
3	2	1	←	3	1	3	3422.5758	0.0004
4	2	2	←	4	1	4	3478.3104	-0.0002
6	1	6	←	5	1	5	3528.2004	0.0012
5	2	3	←	5	1	5	3551.4332	0.0008
6	4	2	←	7	3	4	3585.8966	0.0157
6	4	3	←	7	3	5	3586.8385	-0.0103
6	0	6	←	5	0	5	3592.6165	0.0010
6	2	5	←	5	2	4	3605.8959	0.0019
6	4	3	←	5	4	2	3609.8842	0.0043
6	3	4	←	5	3	3	3610.3371	0.0018
6	3	3	←	5	3	2	3610.5961	0.0019
6	2	4	←	5	2	3	3620.9323	0.0017
6	2	4	←	6	1	6	3644.1643	0.0004
4	1	3	←	3	0	3	3647.9625	0.0013
19	3	17	←	18	4	15	3649.9458	0.0003
14	1	14	←	13	2	12	3662.4625	-0.0009
22	3	20	←	22	2	20	3673.8772	0.0079
6	1	5	←	5	1	4	3680.2661	0.0012
9	0	9	←	8	1	7	3721.7897	0.0004
16	2	15	←	15	3	13	3735.0327	-0.0014
7	2	5	←	7	1	7	3759.0613	0.0004
11	1	10	←	10	2	8	3848.8395	0.0003
21	3	19	←	21	2	19	3891.4288	0.0074
8	2	6	←	8	1	8	3898.9171	0.0000
19	3	16	←	18	4	14	3946.6621	0.0001
15	2	13	←	14	3	11	4019.7869	-0.0037
15	1	15	←	14	2	13	4057.0173	-0.0016
9	2	7	←	9	1	9	4066.6345	0.0003
20	3	18	←	20	2	18	4100.2522	0.0064
7	1	7	←	6	1	6	4114.6145	0.0008
10	0	10	←	9	1	8	4155.2462	-0.0022
7	0	7	←	6	0	6	4184.9277	0.0012
5	4	1	←	6	3	3	4189.1777	-0.0100
5	4	2	←	6	3	4	4189.5689	-0.0069
7	2	6	←	6	2	5	4205.6511	0.0024
7	5	2	←	6	5	1	4211.7031	0.0004
7	4	4	←	6	4	3	4211.8331	0.0048
7	6	1	←	6	6	0	4211.9792	-0.0001

7	3	5	←	6	3	4	4212.6094	0.0025
7	3	4	←	6	3	3	4213.1892	0.0009
7	2	5	←	6	2	4	4229.5109	0.0001
20	3	18	←	19	4	16	4242.0259	0.0044
17	2	16	←	16	3	14	4258.3763	-0.0018
10	2	8	←	10	1	10	4265.0673	0.0014
7	1	6	←	6	1	5	4291.7047	0.0021
19	3	17	←	19	2	17	4298.6745	0.0058
5	1	4	←	4	0	4	4315.1049	-0.0005
12	6	6	←	13	5	8	4428.7797	0.0031
16	1	16	←	15	2	14	4437.8324	-0.0016
5	2	4	←	5	0	5	4472.7464	-0.0047
18	3	16	←	18	2	16	4485.1410	0.0056
6	2	5	←	6	0	6	4486.0288	-0.0008
12	1	11	←	11	2	9	4494.6820	0.0015
11	2	9	←	11	1	11	4496.8501	0.0009
2	2	0	←	1	1	0	4534.2570	-0.0008
2	2	1	←	1	1	1	4559.2264	-0.0008
11	0	11	←	10	1	9	4561.7643	0.0004
9	2	8	←	9	0	9	4579.3044	0.0014
20	3	17	←	19	4	15	4631.2553	0.0044
10	2	9	←	10	0	10	4635.5637	0.0147
17	3	15	←	17	2	15	4658.2318	0.0054
8	1	8	←	7	1	7	4700.3456	0.0017
11	2	10	←	11	0	11	4707.7881	0.0015
16	2	14	←	15	3	12	4738.0531	-0.0024
12	2	10	←	12	1	12	4764.2486	0.0014
18	2	17	←	17	3	15	4769.6592	0.0005
8	0	8	←	7	0	7	4774.4977	0.0009
8	2	7	←	7	2	6	4804.8407	0.0009
17	1	17	←	16	2	15	4805.2953	-0.0149
8	5	4	←	7	5	3	4813.5601	0.0026
8	6	2	←	7	6	1	4813.7618	0.0017
8	4	5	←	7	4	4	4813.9240	0.0101
8	7	1	←	7	7	0	4814.2870	0.0010
8	3	6	←	7	3	5	4815.0722	0.0022
8	3	5	←	7	3	4	4816.2317	0.0018
16	3	14	←	16	2	14	4816.6960	0.0044
21	3	19	←	20	4	17	4829.1496	0.0037
8	2	6	←	7	2	5	4840.2013	0.0010
8	1	7	←	7	1	6	4902.1828	0.0021
13	2	12	←	13	0	13	4906.1688	0.0005
12	0	12	←	11	1	10	4940.4391	0.0008
15	3	13	←	15	2	13	4959.5056	0.0064
6	1	5	←	5	0	5	4997.5485	0.0010

11	6	5	←	12	5	7	5031.6850	-0.0054
14	2	13	←	14	0	14	5034.0929	0.0076
13	2	11	←	13	1	13	5069.0294	0.0037
14	3	12	←	14	2	12	5085.9052	0.0025
3	2	1	←	2	1	1	5111.9706	0.0004
13	1	12	←	12	2	10	5124.9021	-0.0018
18	1	18	←	17	2	16	5159.9366	0.0007
3	2	2	←	2	1	2	5186.0093	0.0005
13	3	11	←	13	2	11	5195.5154	0.0009
7	5	2	←	8	4	4	5213.2854	0.0039
19	2	18	←	18	3	16	5268.2072	-0.0007
9	1	9	←	8	1	8	5285.3353	0.0005
12	3	10	←	12	2	10	5288.3734	0.0008
13	0	13	←	12	1	11	5291.0006	0.0001
21	3	18	←	20	4	16	5330.0465	0.0090
16	2	15	←	16	0	16	5348.0832	0.0080
9	0	9	←	8	0	8	5361.1821	0.0007
11	3	9	←	11	2	9	5364.9862	0.0013
9	2	8	←	8	2	7	5403.3903	0.0008
14	2	12	←	14	1	14	5412.3815	0.0020
9	5	5	←	8	5	4	5415.4876	0.0027
9	6	3	←	8	6	2	5415.5695	0.0010
9	7	2	←	8	7	1	5416.0797	0.0049
9	4	5	←	8	4	4	5416.2000	0.0138
9	8	1	←	8	8	0	5416.8668	-0.0008
9	3	7	←	8	3	6	5417.7122	0.0022
9	3	6	←	8	3	5	5419.8317	0.0025
10	3	8	←	10	2	8	5426.3290	-0.0011
14	7	7	←	15	6	9	5452.8188	-0.0025
9	2	7	←	8	2	6	5453.0529	0.0009
17	2	15	←	16	3	13	5461.9396	-0.0027
9	3	7	←	9	2	7	5473.8102	0.0005
19	1	19	←	18	2	17	5502.2800	0.0007
8	3	6	←	8	2	6	5509.1517	-0.0001
9	1	8	←	8	1	7	5511.5168	0.0003
7	3	5	←	7	2	5	5534.2822	0.0003
6	3	4	←	6	2	4	5551.1850	-0.0009
5	3	3	←	5	2	3	5561.7786	-0.0025
4	3	2	←	4	2	2	5567.8132	-0.0029
3	3	1	←	3	2	1	5570.8202	0.0203
3	3	0	←	3	2	2	5572.9650	-0.0087
4	3	1	←	4	2	3	5574.3434	-0.0055
5	3	2	←	5	2	4	5577.0477	-0.0001
6	3	3	←	6	2	5	5581.7485	0.0004
7	3	4	←	7	2	6	5589.2880	0.0004
8	3	5	←	8	2	7	5600.6776	-0.0001

14	0	14	←	13	1	12	5613.8760	0.0000
9	3	6	←	9	2	8	5617.1167	-0.0007
10	3	7	←	10	2	9	5640.0119	0.0020
11	3	8	←	11	2	10	5670.9803	0.0021
4	2	2	←	3	1	2	5679.5142	0.0000
7	1	6	←	6	0	6	5696.6363	0.0017
12	3	9	←	12	2	11	5711.8823	0.0026
14	1	13	←	13	2	11	5736.2472	-0.0011
20	2	19	←	19	3	17	5753.4550	-0.0010
13	3	10	←	13	2	12	5764.8188	0.0018
15	2	13	←	15	1	15	5794.9155	0.0018
6	5	1	←	7	4	3	5815.4986	-0.0076
4	2	3	←	3	1	3	5825.4164	-0.0001
14	3	11	←	14	2	13	5832.1430	0.0011
20	1	20	←	19	2	18	5832.9761	-0.0035
10	1	10	←	9	1	9	5869.5466	0.0006
15	0	15	←	14	1	13	5910.1974	0.0011
15	3	12	←	15	2	14	5916.4510	0.0022
10	0	10	←	9	0	9	5944.9760	0.0005
10	2	9	←	9	2	8	6001.2221	0.0005
10	6	4	←	9	6	3	6017.4125	0.0047
10	5	6	←	9	5	5	6017.4986	0.0045
10	7	3	←	9	7	2	6017.8670	0.0027
10	4	7	←	9	4	6	6018.5640	-0.0004
10	4	6	←	9	4	5	6018.6398	0.0056
10	9	1	←	9	9	0	6019.7586	-0.0028
10	3	8	←	9	3	7	6020.4997	0.0018
10	3	7	←	9	3	6	6024.1150	0.0008
13	7	6	←	14	6	8	6054.9677	-0.0024
10	2	8	←	9	2	7	6067.9787	0.0011
10	1	9	←	9	1	8	6119.5095	-0.0002
17	3	14	←	17	2	16	6147.4468	0.0043
16	0	16	←	15	1	14	6181.7567	0.0020
18	2	16	←	17	3	14	6188.0391	-0.0022
16	2	14	←	16	1	16	6216.6712	0.0008
21	2	20	←	20	3	18	6224.9403	-0.0003
9	6	3	←	10	5	5	6236.3855	-0.0066
5	2	3	←	4	1	3	6238.6412	0.0007
18	3	15	←	18	2	17	6300.2251	0.0030
15	1	14	←	14	2	12	6325.7474	-0.0015
8	1	7	←	7	0	7	6413.8901	0.0013
5	5	0	←	6	4	2	6417.4210	-0.0066
17	0	17	←	16	1	15	6430.9192	0.0010
11	1	11	←	10	1	10	6452.9511	-0.0007
22	1	22	←	21	2	20	6462.2888	0.0025
5	2	4	←	4	1	4	6477.4660	0.0014

19	3	16	←	19	2	18	6482.0156	0.0060
11	0	11	←	10	0	10	6526.0252	-0.0001
11	2	10	←	10	2	9	6598.2629	0.0001
11	6	6	←	10	6	5	6619.2846	0.0037
11	5	7	←	10	5	6	6619.5991	0.0057
11	8	3	←	10	8	2	6620.4668	0.0001
11	4	8	←	10	4	7	6621.1607	0.0019
11	4	7	←	10	4	6	6621.3002	0.0022
11	9	2	←	10	9	1	6621.5992	-0.0037
11	10	1	←	10	10	0	6622.9900	-0.0145
11	3	9	←	10	3	8	6623.3906	0.0007
11	3	8	←	10	3	7	6629.2325	0.0014
18	0	18	←	17	1	16	6660.5117	0.0011
17	2	15	←	17	1	17	6677.1823	-0.0016
22	2	21	←	21	3	19	6682.3145	0.0020
11	2	9	←	10	2	8	6684.7359	0.0007
20	3	17	←	20	2	19	6695.8315	0.0053
11	1	10	←	10	1	9	6725.9422	0.0005
23	1	23	←	22	2	21	6762.4109	0.0005
23	3	20	←	22	4	18	6770.9652	0.0146
6	2	4	←	5	1	4	6791.5375	0.0011
8	6	2	←	9	5	4	6838.3103	-0.0080
19	0	19	←	18	1	17	6873.6761	-0.0004
16	1	15	←	15	2	13	6890.7571	-0.0025
19	2	17	←	18	3	15	6912.5345	-0.0011
21	3	18	←	21	2	20	6944.4669	0.0014
23	4	20	←	23	3	20	7034.8800	0.0010
12	1	12	←	11	1	11	7035.5419	-0.0001
12	0	12	←	11	0	11	7104.6160	0.0000
6	2	5	←	5	1	5	7142.1900	0.0009
9	1	8	←	8	0	8	7150.9099	0.0013
18	2	16	←	18	1	18	7175.5502	0.0024
22	4	19	←	22	3	19	7176.2639	0.0007
12	2	11	←	11	2	10	7194.4426	0.0002
12	6	6	←	11	6	5	7221.1950	0.0036
12	7	5	←	11	7	4	7221.4470	0.0016
12	5	8	←	11	5	7	7221.7959	0.0042
12	8	4	←	11	8	3	7222.2328	-0.0002
12	9	3	←	11	9	2	7223.4010	-0.0048
12	4	9	←	11	4	8	7223.9495	0.0014
12	4	8	←	11	4	7	7224.2112	0.0030
12	10	2	←	11	10	1	7224.8763	-0.0108
12	3	10	←	11	3	9	7226.3288	0.0010
22	3	19	←	22	2	21	7230.3725	0.0088
12	3	9	←	11	3	8	7235.3453	0.0014
11	7	4	←	12	6	6	7258.5641	-0.0023

21	0	21	←	20	1	19	7264.0154	-0.0005
21	4	18	←	21	3	18	7298.5023	0.0044
12	2	10	←	11	2	9	7302.9406	0.0006
12	1	11	←	11	1	10	7330.5769	0.0004
7	2	5	←	6	1	5	7340.7786	-0.0037
3	3	0	←	2	2	0	7376.5858	0.0044
3	3	1	←	2	2	1	7377.0010	-0.0098
20	4	17	←	20	3	17	7402.5018	0.0027
17	1	16	←	16	2	14	7428.9491	-0.0032
7	6	1	←	8	5	3	7440.0297	-0.0136
19	4	16	←	19	3	16	7489.5602	-0.0003
18	4	15	←	18	3	15	7561.2592	0.0003
13	1	13	←	12	1	12	7617.3181	-0.0015
17	4	14	←	17	3	14	7619.3471	0.0022
20	2	18	←	19	3	16	7631.3341	-0.0021
16	4	13	←	16	3	13	7665.6338	-0.0003
14	8	6	←	15	7	8	7678.5576	0.0111
13	0	13	←	12	0	12	7681.1384	-0.0003
15	4	12	←	15	3	12	7701.9105	-0.0013
14	4	11	←	14	3	11	7729.8586	-0.0011
13	4	10	←	13	3	10	7751.0043	-0.0018
12	4	9	←	12	3	9	7766.6967	-0.0016
11	4	8	←	11	3	8	7778.0923	-0.0018
10	4	7	←	10	3	7	7786.1645	-0.0018
14	4	10	←	14	3	12	7786.9724	-0.0015
15	4	11	←	15	3	13	7787.1298	-0.0015
13	4	9	←	13	3	11	7788.1012	-0.0013
16	4	12	←	16	3	14	7789.3087	-0.0004
13	2	12	←	12	2	11	7789.6945	0.0005
12	4	8	←	12	3	10	7789.9412	-0.0013
9	4	6	←	9	3	6	7791.7133	-0.0028
11	4	7	←	11	3	9	7792.0615	-0.0005
10	4	6	←	10	3	8	7794.1514	-0.0024
17	4	13	←	17	3	15	7794.4159	-0.0008
8	4	5	←	8	3	5	7795.3847	-0.0066
9	4	5	←	9	3	7	7796.0150	-0.0025
8	4	4	←	8	3	6	7797.5422	0.0010
7	4	4	←	7	3	4	7797.6886	-0.0187
7	4	3	←	7	3	5	7798.6975	0.0136
6	4	3	←	6	3	3	7799.0379	-0.0294
6	4	2	←	6	3	4	7799.4531	-0.0045
5	4	2	←	5	3	2	7799.7922	0.0106
5	4	1	←	5	3	3	7799.8827	-0.0288
4	4	1	←	4	3	1	7800.0960	0.0114
18	4	14	←	18	3	16	7803.5550	-0.0005
19	4	15	←	19	3	17	7818.0319	0.0006

7	2	6	←	6	1	6	7819.6386	-0.0002
13	6	8	←	12	6	7	7823.1427	0.0008
13	7	6	←	12	7	5	7823.2377	0.0012
13	8	5	←	12	8	4	7823.9718	-0.0023
13	5	9	←	12	5	8	7824.1032	0.0059
13	9	4	←	12	9	3	7825.1608	-0.0052
13	10	3	←	12	10	2	7826.7013	-0.0136
13	4	10	←	12	4	9	7826.9411	0.0020
13	4	9	←	12	4	8	7827.4013	0.0015
13	3	11	←	12	3	10	7829.2389	-0.0010
20	4	16	←	20	3	18	7839.3667	-0.0019
13	3	10	←	12	3	9	7842.6317	0.0005
10	7	3	←	11	6	5	7860.1003	-0.0028
21	4	17	←	21	3	19	7869.3175	-0.0025
8	2	6	←	7	1	6	7889.2799	0.0001
10	1	9	←	9	0	9	7909.2373	0.0005
22	4	18	←	22	3	20	7909.8725	-0.0022
13	2	11	←	12	2	10	7922.0978	-0.0002
13	1	12	←	12	1	11	7933.1618	-0.0016
18	1	17	←	17	2	15	7938.3114	0.0000
23	4	19	←	23	3	21	7963.2573	-0.0041
4	3	1	←	3	2	1	7977.1877	-0.0024
4	3	2	←	3	2	2	7979.3249	-0.0019
2	1	2	←	1	0	1	2279.2158	-0.0003
12	1	11	←	12	0	12	2390.1536	0.0154
9	1	8	←	8	2	7	2613.8132	-0.0005
13	1	12	←	13	0	13	2642.1603	-0.0026
13	2	11	←	13	1	12	2797.1965	0.0023
14	2	12	←	14	1	13	2805.4133	0.0074
12	2	10	←	12	1	11	2808.2759	0.0165
15	2	13	←	15	1	14	2835.2971	0.0006
11	2	9	←	11	1	10	2835.8961	0.0002
3	1	3	←	2	0	2	2842.6073	0.0012
10	2	8	←	10	1	9	2877.1041	0.0016
14	1	13	←	14	0	14	2919.5688	0.0023
9	2	7	←	9	1	8	2928.6311	-0.0035
17	2	15	←	17	1	16	2968.3253	-0.0061
7	4	4	←	8	3	5	2981.4818	0.0044
8	2	6	←	8	1	7	2987.0999	0.0008
7	2	5	←	7	1	6	3049.0790	-0.0006
18	2	16	←	18	1	17	3074.9619	0.0034
6	2	4	←	6	1	5	3111.2727	0.0012
15	2	14	←	14	3	11	3145.0294	-0.0007
3	3	1	←	4	2	2	3161.4717	0.0133
3	3	0	←	4	2	3	3167.9659	0.0025
5	2	3	←	5	1	4	3170.6036	-0.0022

19	2	17	←	19	1	18	3210.2359	0.0078
15	1	14	←	15	0	15	3220.9536	-0.0048
14	6	9	←	15	5	10	3221.4677	0.0398
4	2	2	←	4	1	3	3224.3499	0.0007
3	2	1	←	3	1	2	3270.1734	0.0007
2	2	0	←	2	1	1	3306.1922	-0.0011
7	0	7	←	6	1	6	3312.8905	0.0036
2	2	1	←	2	1	2	3381.9641	-0.0029
4	1	4	←	3	0	3	3393.9995	-0.0004
10	5	6	←	11	4	7	3403.6908	-0.0085
10	5	5	←	11	4	8	3403.9713	0.0094
3	2	2	←	3	1	3	3420.4061	-0.0001
4	2	3	←	4	1	4	3471.8108	0.0007
5	2	4	←	5	1	5	3536.2964	0.0012
16	1	15	←	16	0	16	3544.2746	-0.0268
6	2	5	←	6	1	6	3613.9878	-0.0022
7	2	6	←	7	1	7	3705.0301	0.0051
8	2	7	←	8	1	8	3809.5145	-0.0064
13	6	8	←	14	5	9	3825.3920	0.0076
9	2	8	←	9	1	9	3927.5782	0.0027
5	1	5	←	4	0	4	3934.2802	0.0014
8	0	8	←	7	1	7	3972.7677	-0.0023
11	1	10	←	10	2	9	4054.6430	-0.0109
10	2	9	←	10	1	10	4059.2543	0.0031
11	2	10	←	11	1	11	4204.5581	-0.0040
12	2	11	←	12	1	12	4363.4635	0.0009
6	1	6	←	5	0	5	4464.6569	0.0018
2	2	1	←	1	1	0	4533.8243	0.0006
2	2	0	←	1	1	1	4559.6585	-0.0028
9	0	9	←	8	1	8	4633.6059	-0.0015
14	2	13	←	14	1	14	4721.4886	-0.0038
12	1	11	←	11	2	10	4786.9718	0.0042
17	3	14	←	17	2	15	4825.2322	0.0036
15	2	14	←	15	1	15	4920.1499	-0.0033
16	3	13	←	16	2	14	4935.3239	-0.0175
7	1	7	←	6	0	6	4986.6548	0.0015
15	3	12	←	15	2	13	5041.6888	0.0005
3	2	2	←	2	1	1	5109.8007	-0.0004
16	2	15	←	16	1	16	5131.4658	0.0059
14	3	11	←	14	2	12	5141.2649	0.0101
3	2	1	←	2	1	2	5188.1776	-0.0004
7	5	3	←	8	4	4	5213.2854	0.0039
13	3	10	←	13	2	11	5231.6071	-0.0211
10	0	10	←	9	1	9	5293.2485	0.0004
12	3	9	←	12	2	10	5311.0959	0.0008
10	3	7	←	10	2	8	5434.1924	-0.0028

9	3	6	←	9	2	7	5478.0552	-0.0034
8	1	8	←	7	0	7	5502.0713	0.0005
8	3	5	←	8	2	6	5511.2824	0.0010
13	1	12	←	12	2	11	5525.6760	-0.0125
7	3	4	←	7	2	5	5535.2530	0.0012
6	3	3	←	6	2	4	5551.5736	-0.0006
5	3	2	←	5	2	3	5561.9096	-0.0011
4	3	1	←	4	2	2	5567.8332	-0.0153
3	3	0	←	3	2	1	5570.8202	0.0157
3	3	1	←	3	2	2	5572.9650	-0.0040
4	3	2	←	4	2	3	5574.3441	0.0275
5	3	3	←	5	2	4	5576.9187	0.0005
6	3	4	←	6	2	5	5581.3602	0.0005
7	3	5	←	7	2	6	5588.3150	-0.0029
8	3	6	←	8	2	7	5598.5487	0.0007
9	3	7	←	9	2	8	5612.8666	-0.0020
10	3	8	←	10	2	9	5632.1445	-0.0003
11	3	9	←	11	2	10	5657.2715	-0.0004
4	2	3	←	3	1	2	5673.0142	0.0004
12	3	10	←	12	2	11	5689.1610	0.0037
13	3	11	←	13	2	12	5728.7016	-0.0016
14	3	12	←	14	2	13	5776.7908	0.0009
6	5	2	←	7	4	3	5815.4986	-0.0076
4	2	2	←	3	1	3	5831.9173	0.0005
15	3	13	←	15	2	14	5834.2563	-0.0034
16	3	14	←	16	2	15	5901.8841	-0.0180
11	0	11	←	10	1	10	5949.7261	-0.0012
9	1	9	←	8	0	8	6012.9114	0.0025
18	3	16	←	18	2	17	6070.5054	-0.0146
5	2	4	←	4	1	3	6223.5036	0.0003
14	1	13	←	13	2	12	6269.4362	-0.0008
5	2	3	←	4	1	4	6492.6023	0.0005
10	1	10	←	9	0	9	6521.2753	0.0019
12	0	12	←	11	1	11	6601.3945	0.0030
6	2	5	←	5	1	4	6761.3618	-0.0008
15	1	14	←	14	2	13	7016.6272	-0.0088
11	1	11	←	10	0	10	7029.2507	0.0009
6	2	4	←	5	1	5	7172.3605	-0.0024
13	0	13	←	12	1	12	7246.9876	-0.0007
7	2	6	←	6	1	5	7286.7474	0.0010
3	3	1	←	2	2	0	7376.5858	0.0091
3	3	0	←	2	2	1	7377.0010	-0.0144
12	1	12	←	11	0	11	7538.7675	0.0010
16	4	12	←	16	3	13	7670.6499	-0.0094
15	4	11	←	15	3	12	7704.9430	0.0007
14	4	10	←	14	3	11	7731.6203	-0.0016

13	4	9	←	13	3	10	7751.9922	0.0036
12	4	8	←	12	3	9	7767.2199	-0.0002
11	4	7	←	11	3	8	7778.3495	-0.0063
15	4	12	←	15	3	13	7784.1012	0.0003
16	4	13	←	16	3	14	7784.2846	0.0008
14	4	11	←	14	3	12	7785.2196	0.0079
10	4	6	←	10	3	7	7786.2857	-0.0031
12	4	9	←	12	3	10	7789.4048	-0.0159
9	4	5	←	9	3	6	7791.7524	-0.0163
10	4	7	←	10	3	8	7794.0306	-0.0009
8	4	4	←	8	3	5	7795.3847	-0.0269
9	4	6	←	9	3	7	7795.9825	0.0175
8	4	5	←	8	3	6	7797.5422	0.0212
7	4	3	←	7	3	4	7797.6886	-0.0255
7	4	4	←	7	3	5	7798.6975	0.0204
6	4	2	←	6	3	3	7799.0939	0.0247
6	4	3	←	6	3	4	7799.4531	-0.0027
5	4	1	←	5	3	2	7799.7922	0.0102
8	2	7	←	7	1	6	7799.8827	-0.0009
4	4	0	←	4	3	1	7800.0960	0.0114
7	2	5	←	6	1	6	7873.6715	-0.0031
14	0	14	←	13	1	13	7885.7033	-0.0043
4	3	2	←	3	2	1	7977.1577	0.0000
4	3	1	←	3	2	2	7979.3449	-0.0144
							RMS	**6.39 kHz**

Table S10. List of assigned transitions for phenol dimer, $^{13}C(1)$ isotopologue

J'	K_a '	K_c '	←	J''	K_a''	K_c ''	ν_{obs} (MHz)	ν_{obs} - ν_{calc}
4	1	4	←	3	1	3	2347.1463	0.0010
4	0	4	←	3	0	3	2394.3411	-0.0014
4	2	3	←	3	2	2	2398.4565	0.0047
4	2	2	←	3	2	1	2402.7729	0.0008
4	1	3	←	3	1	2	2448.5108	-0.0017
7	0	7	←	6	1	5	2770.5257	-0.0193
8	2	7	←	8	1	7	2894.3921	0.0102
5	1	5	←	4	1	4	2933.0970	0.0014
3	1	2	←	2	0	2	2988.5579	0.0171
5	0	5	←	4	0	4	2989.6459	-0.0005
7	2	6	←	7	1	6	2991.5477	0.0060
5	2	4	←	4	2	3	2997.4588	0.0008
5	4	1	←	4	4	0	2999.8588	0.0113
5	3	2	←	4	3	1	3000.1481	-0.0018
5	2	3	←	4	2	2	3006.0794	0.0062
5	1	4	←	4	1	3	3059.7446	0.0232
5	2	4	←	5	1	4	3151.6704	0.0036
4	2	3	←	4	1	3	3213.9276	-0.0026
3	2	2	←	3	1	2	3263.9868	-0.0041
3	2	1	←	3	1	3	3418.2722	0.0021
4	2	2	←	4	1	4	3473.8922	-0.0047
6	1	6	←	5	1	5	3518.5142	0.0003
6	0	6	←	5	0	5	3582.8152	-0.0006
6	2	5	←	5	2	4	3596.0613	0.0006
6	4	3	←	5	4	2	3600.0351	-0.0007
6	3	4	←	5	3	3	3600.4939	0.0032
6	3	3	←	5	3	2	3600.7468	-0.0019
6	2	4	←	5	2	3	3611.0583	-0.0015
6	2	4	←	6	1	6	3639.4409	0.0205
4	1	3	←	3	0	3	3639.7394	-0.0164
6	1	5	←	5	1	4	3670.2901	-0.0025
8	2	6	←	8	1	8	3893.6416	-0.0107
7	1	7	←	6	1	6	4103.3201	0.0013
7	0	7	←	6	0	6	4173.5095	-0.0005
7	2	6	←	6	2	5	4194.1784	-0.0015
7	5	2	←	6	5	1	4200.2288	0.0118
7	4	4	←	6	4	3	4200.3448	0.0017
7	3	5	←	6	3	4	4201.1211	0.0007
7	3	4	←	6	3	3	4201.6993	-0.0007
7	2	5	←	6	2	4	4217.9789	-0.0036
7	1	6	←	6	1	5	4280.0700	-0.0032

5	1	4	←	4	0	4	4305.1418	0.0072
2	2	1	←	1	1	1	4551.7622	-0.0061
8	1	8	←	7	1	7	4687.4414	0.0001
8	0	8	←	7	0	7	4761.4705	0.0005
8	2	7	←	7	2	6	4791.7364	-0.0007
8	5	3	←	7	5	2	4800.4268	-0.0042
8	6	2	←	7	6	1	4800.6198	-0.0123
8	4	5	←	7	4	4	4800.7914	0.0041
8	3	6	←	7	3	5	4801.9400	-0.0014
8	3	5	←	7	3	4	4803.0970	-0.0007
8	2	6	←	7	2	5	4827.0077	-0.0019
8	1	7	←	7	1	6	4888.8941	-0.0028
6	1	5	←	5	0	5	4985.7896	0.0088
3	2	1	←	2	1	1	5102.9640	0.0024
3	2	2	←	2	1	2	5176.8604	-0.0017
9	1	9	←	8	1	8	5270.8261	-0.0005
9	0	9	←	8	0	8	5346.5508	-0.0006
9	2	8	←	8	2	7	5388.6541	-0.0005
9	5	5	←	8	5	4	5400.7135	-0.0040
9	6	4	←	8	6	3	5400.8004	0.0007
9	4	5	←	8	4	4	5401.4250	0.0071
9	3	7	←	8	3	6	5402.9389	-0.0003
9	3	6	←	8	3	5	5405.0507	-0.0010
9	1	8	←	8	1	7	5496.5788	-0.0026
7	3	5	←	7	2	5	5527.6494	0.0044
4	2	2	←	3	1	2	5668.9226	-0.0042
7	1	6	←	6	0	6	5683.0431	0.0049
4	2	3	←	3	1	3	5814.5328	-0.0254
10	1	10	←	9	1	9	5853.4330	-0.0012
10	0	10	←	9	0	9	5928.7505	0.0016
10	2	9	←	9	2	8	5984.8549	-0.0017
10	6	5	←	9	6	4	6001.0006	0.0023
10	5	6	←	9	5	5	6001.0843	-0.0014
10	4	7	←	9	4	6	6002.1511	-0.0033
10	4	6	←	9	4	5	6002.2255	0.0016
10	3	8	←	9	3	7	6004.0843	-0.0005
10	3	7	←	9	3	6	6007.7155	0.0259
10	2	8	←	9	2	7	6051.4468	-0.0022
10	1	9	←	9	1	8	6102.9262	-0.0007
5	2	3	←	4	1	3	6226.4654	-0.0221
8	1	7	←	7	0	7	6398.4330	0.0079
11	1	11	←	10	1	10	6435.2389	0.0000
11	0	11	←	10	0	10	6508.2088	0.0011
11	2	10	←	10	2	9	6580.2718	0.0019
11	5	7	←	10	5	6	6601.5488	0.0047
11	4	8	←	10	4	7	6603.0978	-0.0089

11	4	7	←	10	4	6	6603.2500	0.0047
11	3	9	←	10	3	8	6605.3336	-0.0010
11	3	8	←	10	3	7	6611.1568	-0.0005
11	2	9	←	10	2	8	6666.5305	-0.0020
11	1	10	←	10	1	9	6707.7153	-0.0002
6	2	4	←	5	1	4	6777.8229	-0.0029
12	1	12	←	11	1	11	7016.2294	-0.0008
12	0	12	←	11	0	11	7085.2144	0.0021
6	2	5	←	5	1	5	7127.8221	-0.0139
9	1	8	←	8	0	8	7133.5301	-0.0064
12	2	11	←	11	2	10	7174.8246	0.0006
12	5	8	←	11	5	7	7202.1012	-0.0001
12	4	9	←	11	4	8	7204.2184	-0.0351
12	4	8	←	11	4	7	7204.5125	-0.0002
12	3	10	←	11	3	9	7206.6292	-0.0013
12	3	9	←	11	3	8	7215.6194	0.0013
12	2	10	←	11	2	9	7283.0614	-0.0002
12	1	11	←	11	1	10	7310.7141	0.0022
7	2	5	←	6	1	5	7325.5459	0.0302
13	1	13	←	12	1	12	7596.4090	-0.0022
13	0	13	←	12	0	12	7660.1529	0.0004
13	2	12	←	12	2	11	7768.4536	0.0009
13	6	8	←	12	6	7	7801.8145	0.0032
13	7	6	←	12	7	5	7801.9001	-0.0035
13	5	9	←	12	5	8	7802.7735	0.0078
13	4	10	←	12	4	9	7805.5919	-0.0099
13	4	9	←	12	4	8	7806.0670	0.0062
13	3	11	←	12	3	10	7807.9048	0.0036
13	3	10	←	12	3	9	7821.2530	0.0027
8	2	6	←	7	1	6	7872.4536	0.0015
10	1	9	←	9	0	9	7889.9143	0.0025
13	2	11	←	12	2	10	7900.5464	0.0026
13	1	12	←	12	1	11	7911.6714	0.0051
							RMS	**8.08 kHz**

Table S11. List of assigned transitions for phenol dimer, $^{13}C(2)$ isotopologue.

J'	K_a '	K_c '	←	J''	K_a''	K_c ''	ν_{obs} (MHz)	ν_{obs} - ν_{calc}
4	1	4	←	3	1	3	2349.7939	0.0004
2	1	1	←	1	0	1	2351.0021	-0.0006
4	0	4	←	3	0	3	2396.7638	0.0014
4	1	3	←	3	1	2	2450.6364	-0.0008
5	1	5	←	4	1	4	2936.4142	0.0015
3	1	2	←	2	0	2	2989.2717	-0.0004
5	0	5	←	4	0	4	2992.7014	-0.0006
5	2	4	←	4	2	3	3000.4392	-0.0005
5	3	3	←	4	3	2	3003.0028	-0.0087
5	3	2	←	4	3	1	3003.1083	0.0013
5	2	3	←	4	2	2	3008.9717	0.0002
5	1	4	←	4	1	3	3062.3846	-0.0009
6	2	5	←	6	1	5	3076.7552	0.0096
5	2	4	←	5	1	4	3150.6076	0.0062
4	2	3	←	4	1	3	3212.5463	-0.0009
3	2	2	←	3	1	2	3262.3519	0.0006
2	2	1	←	2	1	1	3299.8215	-0.0207
3	2	1	←	3	1	3	3415.8152	-0.0082
4	2	2	←	4	1	4	3471.1306	-0.0109
6	1	6	←	5	1	5	3522.5050	0.0006
5	2	3	←	5	1	5	3543.6943	-0.0059
6	0	6	←	5	0	5	3586.5269	0.0004
6	2	5	←	5	2	4	3599.6472	0.0014
6	4	3	←	5	4	2	3603.5924	0.0043
6	3	4	←	5	3	3	3604.0358	0.0000
6	3	3	←	5	3	2	3604.2913	0.0012
6	2	4	←	5	2	3	3614.5018	0.0015
6	2	4	←	6	1	6	3635.6918	-0.0042
4	1	3	←	3	0	3	3640.8099	-0.0012
6	1	5	←	5	1	4	3673.5012	-0.0005
7	2	5	←	7	1	7	3749.6612	0.0052
9	2	7	←	9	1	9	4054.6430	0.0126
7	1	7	←	6	1	6	4107.9902	0.0027
7	0	7	←	6	0	6	4177.8979	0.0004
7	2	6	←	6	2	5	4198.3736	0.0009
7	5	2	←	6	5	1	4204.3589	-0.0038
7	4	4	←	6	4	3	4204.4866	0.0041
7	3	5	←	6	3	4	4205.2507	0.0010
7	3	4	←	6	3	3	4205.8212	0.0002
7	2	5	←	6	2	4	4221.9471	-0.0004
7	1	6	←	6	1	5	4283.8355	0.0008

5	1	4	←	4	0	4	4306.4345	0.0004
2	2	0	←	1	1	0	4526.0594	-0.0067
2	2	1	←	1	1	1	4550.8659	0.0040
8	1	8	←	7	1	7	4692.7948	0.0014
8	0	8	←	7	0	7	4766.5545	-0.0028
8	2	7	←	7	2	6	4796.5411	-0.0008
8	5	4	←	7	5	3	4805.1540	-0.0105
8	4	5	←	7	4	4	4805.5209	0.0091
8	3	6	←	7	3	5	4806.6550	0.0023
8	3	5	←	7	3	4	4807.7949	0.0024
8	2	6	←	7	2	5	4831.4801	-0.0004
8	1	7	←	7	1	6	4893.2194	-0.0004
6	1	5	←	5	0	5	4987.2330	-0.0008
3	2	1	←	2	1	1	5102.8868	-0.0040
3	2	2	←	2	1	2	5176.4178	-0.0013
9	1	9	←	8	1	8	5276.8676	0.0002
9	0	9	←	8	0	8	5352.3599	-0.0002
9	2	8	←	8	2	7	5394.0759	-0.0007
9	5	4	←	8	5	3	5406.0391	0.0016
9	4	5	←	8	4	4	5406.7346	0.0102
9	3	7	←	8	3	6	5408.2300	-0.0006
9	3	6	←	8	3	5	5410.3144	0.0013
9	2	7	←	8	2	6	5443.1528	-0.0018
9	3	7	←	9	2	7	5464.6997	0.0001
8	3	6	←	8	2	6	5499.6276	0.0040
9	1	8	←	8	1	7	5501.4736	-0.0030
7	3	5	←	7	2	5	5524.4569	0.0055
6	3	4	←	6	2	4	5541.1487	-0.0005
5	3	2	←	5	2	4	5566.6931	-0.0009
6	3	3	←	6	2	5	5571.3360	-0.0023
7	3	4	←	7	2	6	5578.7821	-0.0045
8	3	5	←	8	2	7	5590.0360	-0.0013
9	3	6	←	9	2	8	5606.2838	0.0099
10	3	7	←	10	2	9	5628.8721	-0.0088
4	2	2	←	3	1	2	5669.6044	-0.0011
7	1	6	←	6	0	6	5684.5378	-0.0043
4	2	3	←	3	1	3	5814.5328	0.0190
10	1	10	←	9	1	9	5860.1702	0.0012
10	0	10	←	9	0	9	5935.2973	-0.0005
10	2	9	←	9	2	8	5990.9015	0.0000
10	6	4	←	9	6	3	6006.9085	-0.0034
10	4	7	←	9	4	6	6008.0425	0.0013
10	4	6	←	9	4	5	6008.1059	-0.0035
10	3	8	←	9	3	7	6009.9541	-0.0005
10	3	7	←	9	3	6	6013.5083	-0.0003
10	2	8	←	9	2	7	6056.8844	-0.0006

10	1	9	←	9	1	8	6108.4050	-0.0025
5	2	3	←	4	1	3	6227.9390	-0.0007
8	1	7	←	7	0	7	6399.8655	0.0011
11	1	11	←	10	1	10	6442.6735	0.0008
5	2	4	←	4	1	4	6465.1596	-0.0004
11	0	11	←	10	0	10	6515.5106	-0.0005
11	2	10	←	10	2	9	6586.9425	-0.0014
11	6	5	←	10	6	4	6607.7093	-0.0204
11	5	7	←	10	5	6	6608.0310	0.0009
11	7	4	←	10	7	3	6608.0923	-0.0162
11	4	8	←	10	4	7	6609.5737	0.0033
11	4	7	←	10	4	6	6609.7160	0.0095
11	3	9	←	10	3	8	6611.7819	-0.0001
11	3	8	←	10	3	7	6617.5227	-0.0001
11	2	9	←	10	2	8	6672.4341	-0.0026
11	1	10	←	10	1	9	6713.7941	-0.0029
6	2	4	←	5	1	4	6780.0566	0.0020
12	1	12	←	11	1	11	7024.3678	0.0001
12	0	12	←	11	0	11	7093.2782	-0.0003
6	2	5	←	5	1	5	7128.3970	0.0039
9	1	8	←	8	0	8	7134.7840	0.0003
12	2	11	←	11	2	10	7182.1329	-0.0010
12	6	6	←	11	6	5	7208.5862	0.0031
12	5	8	←	11	5	7	7209.1701	0.0029
12	4	9	←	11	4	8	7211.2917	0.0007
12	4	8	←	11	4	7	7211.5456	0.0002
12	3	10	←	11	3	9	7213.6554	-0.0001
12	3	9	←	11	3	8	7222.5160	-0.0012
12	2	10	←	11	2	9	7289.4293	-0.0038
12	1	11	←	11	1	10	7317.4100	-0.0025
7	2	5	←	6	1	5	7328.5026	0.0022
13	1	13	←	12	1	12	7605.2553	-0.0015
13	0	13	←	12	0	12	7668.9834	-0.0001
9	4	6	←	9	3	6	7777.4223	-0.0210
11	4	7	←	11	3	9	7777.7563	0.0070
10	4	6	←	10	3	8	7779.8368	0.0120
7	2	6	←	6	1	6	7804.2554	-0.0060
13	6	8	←	12	6	7	7809.4793	0.0044
13	7	6	←	12	7	5	7809.5834	0.0035
13	5	9	←	12	5	8	7810.4129	0.0039
13	4	10	←	12	4	9	7813.2331	0.0231
13	4	9	←	12	4	8	7813.6562	-0.0043
13	3	11	←	12	3	10	7815.5043	-0.0001
13	3	10	←	12	3	9	7828.6651	-0.0026
8	2	6	←	7	1	6	7876.1485	0.0022

13	2	11	←	12	2	10	7907.3827	-0.0056
13	1	12	←	12	1	11	7919.0046	-0.0017
4	3	1	←	3	2	1	7962.7119	-0.0052
4	3	2	←	3	2	2	7964.8382	0.0103
							RMS	**5.77 kHz**

Table S12. List of assigned transitions for phenol dimer, ^{13}C(3) isotopologue.

J'	K_a '	K_c '	←	J''	K_a''	K_c ''	ν_{obs} (MHz)	ν_{obs} - ν_{calc}
4	1	4	←	3	1	3	2343.5122	-0.0005
4	0	4	←	3	0	3	2390.5346	0.0004
4	2	3	←	3	2	2	2394.6452	-0.0020
4	2	2	←	3	2	1	2398.9686	-0.0035
4	1	3	←	3	1	2	2444.5323	-0.0033
5	1	5	←	4	1	4	2928.5532	-0.0002
3	1	2	←	2	0	2	2976.6517	0.0023
5	0	5	←	4	0	4	2984.8826	0.0004
5	2	4	←	4	2	3	2992.7014	0.0000
5	3	3	←	4	3	2	2995.2964	-0.0007
5	3	2	←	4	3	1	2995.3936	-0.0010
5	2	3	←	4	2	2	3001.3264	0.0012
5	1	4	←	4	1	3	3054.7477	-0.0013
6	1	6	←	5	1	5	3513.0624	0.0011
6	0	6	←	5	0	5	3577.0939	0.0003
6	2	5	←	5	2	4	3590.3505	-0.0007
6	4	3	←	5	4	2	3594.3278	0.0018
6	3	4	←	5	3	3	3594.7809	-0.0025
6	3	3	←	5	3	2	3595.0427	-0.0001
6	2	4	←	5	2	3	3605.3638	-0.0011
4	1	3	←	3	0	3	3626.7419	0.0002
6	1	5	←	5	1	4	3664.3224	-0.0012
7	1	7	←	6	1	6	4096.9576	0.0026
10	0	10	←	9	1	8	4142.8651	0.0212
7	0	7	←	6	0	6	4166.8281	0.0001
7	2	6	←	6	2	5	4187.5158	-0.0013
7	5	2	←	6	5	1	4193.5438	-0.0074
7	4	4	←	6	4	3	4193.7072	0.0261
7	3	5	←	6	3	4	4194.4611	-0.0001
7	3	4	←	6	3	3	4195.0435	-0.0003
7	2	5	←	6	2	4	4211.3403	-0.0009
7	1	6	←	6	1	5	4273.1036	-0.0026
5	1	4	←	4	0	4	4290.9577	0.0011

8	1	8	←	7	1	7	4680.1660	0.0005
8	0	8	←	7	0	7	4753.8284	0.0009
8	2	7	←	7	2	6	4784.1186	-0.0012
8	5	4	←	7	5	3	4792.8120	0.0000
8	6	2	←	7	6	1	4793.0344	0.0264
8	4	5	←	7	4	4	4793.1787	0.0056
8	3	6	←	7	3	5	4794.3282	-0.0014
8	3	5	←	7	3	4	4795.4900	-0.0020
8	2	6	←	7	2	5	4819.4204	-0.0006
8	1	7	←	7	1	6	4880.9275	-0.0025
12	0	12	←	11	1	10	4924.5999	-0.0298
6	1	5	←	5	0	5	4970.4010	0.0030
9	1	9	←	8	1	8	5262.6419	0.0040
9	0	9	←	8	0	8	5337.9508	0.0012
9	2	8	←	8	2	7	5380.0800	-0.0019
9	5	4	←	8	5	3	5392.1401	-0.0053
9	6	3	←	8	6	2	5392.2205	-0.0010
9	4	5	←	8	4	4	5392.8592	0.0078
9	3	7	←	8	3	6	5394.3718	-0.0021
9	3	6	←	8	3	5	5396.4957	-0.0021
9	2	7	←	8	2	6	5429.6544	-0.0011
9	1	8	←	8	1	7	5487.6090	-0.0031
7	1	6	←	6	0	6	5666.4068	-0.0037
4	2	3	←	3	1	3	5784.0726	-0.0263
10	1	10	←	9	1	9	5844.3365	0.0045
10	0	10	←	9	0	9	5919.1955	0.0040
10	2	9	←	9	2	8	5975.3268	-0.0007
10	6	5	←	9	6	4	5991.4661	0.0007
10	5	6	←	9	5	5	5991.5579	-0.0016
10	7	3	←	9	7	2	5991.9252	0.0133
10	4	7	←	9	4	6	5992.6210	-0.0138
10	4	6	←	9	4	5	5992.6691	-0.0359
10	3	8	←	9	3	7	5994.5619	-0.0029
10	3	7	←	9	3	6	5998.1889	0.0001
10	2	8	←	9	2	7	6041.9522	-0.0016
10	1	9	←	9	1	8	6092.9488	-0.0035
8	1	7	←	7	0	7	6380.4956	-0.0170
11	1	11	←	10	1	10	6425.2322	0.0095
5	2	4	←	4	1	4	6433.2888	0.0013
11	0	11	←	10	0	10	6497.7082	0.0064
11	2	10	←	10	2	9	6569.7813	-0.0016
11	6	5	←	10	6	4	6590.7393	-0.0037
11	5	7	←	10	5	6	6591.0658	0.0020
11	4	8	←	10	4	7	6592.6359	0.0021
11	4	7	←	10	4	6	6592.7681	-0.0057
11	3	9	←	10	3	8	6594.8533	-0.0049

11	3	8	←	10	3	7	6600.7130	0.0012
11	2	9	←	10	2	8	6656.0709	-0.0007
11	1	10	←	10	1	9	6696.7288	-0.0031
12	1	12	←	11	1	11	7005.3107	0.0111
12	0	12	←	11	0	11	7073.7767	0.0086
6	2	5	←	5	1	5	7095.0847	-0.0007
9	1	8	←	8	0	8	7114.2866	-0.0106
12	2	11	←	11	2	10	7163.3774	-0.0006
12	6	7	←	11	6	6	7190.0631	0.0058
12	7	5	←	11	7	4	7190.2917	-0.0081
12	5	8	←	11	5	7	7190.6679	0.0015
12	4	9	←	11	4	8	7192.8239	-0.0029
12	4	8	←	11	4	7	7193.0866	-0.0020
12	3	10	←	11	3	9	7195.1923	-0.0034
12	3	9	←	11	3	8	7204.2184	-0.0121
12	2	10	←	11	2	9	7271.6220	-0.0001
7	2	5	←	6	1	5	7293.4242	0.0102
12	1	11	←	11	1	10	7298.7126	-0.0024
13	1	13	←	12	1	12	7584.5798	0.0137
13	0	13	←	12	0	12	7647.7953	0.0129
13	2	12	←	12	2	11	7756.0529	0.0066
7	2	6	←	6	1	6	7769.5477	0.0067
13	6	8	←	12	6	7	7789.4048	-0.0067
13	5	9	←	12	5	8	7790.3770	0.0011
13	4	10	←	12	4	9	7793.2178	-0.0031
13	4	9	←	12	4	8	7793.6839	-0.0003
13	3	11	←	12	3	10	7795.5044	-0.0011
13	3	10	←	12	3	9	7808.9268	0.0031
8	2	6	←	7	1	6	7839.7377	0.0088
10	1	9	←	9	0	9	7869.3175	0.0176
13	2	11	←	12	2	10	7888.1095	-0.0004
13	1	12	←	12	1	11	7898.6475	-0.0031
							RMS	**8.25 kHz**

Table S13. List of assigned transitions for phenol dimer, $^{13}C(3)$ isotopologue.

J'	K_a '	K_c '	←	J''	K_a''	K_c ''	ν_{obs} (MHz)	ν_{obs} - ν_{calc}
4	1	4	←	3	1	3	2343.5122	-0.0005
4	0	4	←	3	0	3	2390.5346	0.0004
4	2	3	←	3	2	2	2394.6452	-0.0020
4	2	2	←	3	2	1	2398.9686	-0.0035
4	1	3	←	3	1	2	2444.5323	-0.0033
5	1	5	←	4	1	4	2928.5532	-0.0002
3	1	2	←	2	0	2	2976.6517	0.0023
5	0	5	←	4	0	4	2984.8826	0.0004
5	2	4	←	4	2	3	2992.7014	0.0000
5	3	3	←	4	3	2	2995.2964	-0.0007
5	3	2	←	4	3	1	2995.3936	-0.0010
5	2	3	←	4	2	2	3001.3264	0.0012
5	1	4	←	4	1	3	3054.7477	-0.0013
6	1	6	←	5	1	5	3513.0624	0.0011
6	0	6	←	5	0	5	3577.0939	0.0003
6	2	5	←	5	2	4	3590.3505	-0.0007
6	4	3	←	5	4	2	3594.3278	0.0018
6	3	4	←	5	3	3	3594.7809	-0.0025
6	3	3	←	5	3	2	3595.0427	-0.0001
6	2	4	←	5	2	3	3605.3638	-0.0011
4	1	3	←	3	0	3	3626.7419	0.0002
6	1	5	←	5	1	4	3664.3224	-0.0012
7	1	7	←	6	1	6	4096.9576	0.0026
10	0	10	←	9	1	8	4142.8651	0.0212
7	0	7	←	6	0	6	4166.8281	0.0001
7	2	6	←	6	2	5	4187.5158	-0.0013
7	5	2	←	6	5	1	4193.5438	-0.0074
7	4	4	←	6	4	3	4193.7072	0.0261
7	3	5	←	6	3	4	4194.4611	-0.0001
7	3	4	←	6	3	3	4195.0435	-0.0003
7	2	5	←	6	2	4	4211.3403	-0.0009
7	1	6	←	6	1	5	4273.1036	-0.0026
5	1	4	←	4	0	4	4290.9577	0.0011
8	1	8	←	7	1	7	4680.1660	0.0005
8	0	8	←	7	0	7	4753.8284	0.0009
8	2	7	←	7	2	6	4784.1186	-0.0012
8	5	4	←	7	5	3	4792.8120	0.0000
8	6	2	←	7	6	1	4793.0344	0.0264
8	4	5	←	7	4	4	4793.1787	0.0056
8	3	6	←	7	3	5	4794.3282	-0.0014

8	3	5	←	7	3	4	4795.4900	-0.0020
8	2	6	←	7	2	5	4819.4204	-0.0006
8	1	7	←	7	1	6	4880.9275	-0.0025
12	0	12	←	11	1	10	4924.5999	-0.0298
6	1	5	←	5	0	5	4970.4010	0.0030
9	1	9	←	8	1	8	5262.6419	0.0040
9	0	9	←	8	0	8	5337.9508	0.0012
9	2	8	←	8	2	7	5380.0800	-0.0019
9	5	4	←	8	5	3	5392.1401	-0.0053
9	6	3	←	8	6	2	5392.2205	-0.0010
9	4	5	←	8	4	4	5392.8592	0.0078
9	3	7	←	8	3	6	5394.3718	-0.0021
9	3	6	←	8	3	5	5396.4957	-0.0021
9	2	7	←	8	2	6	5429.6544	-0.0011
9	1	8	←	8	1	7	5487.6090	-0.0031
7	1	6	←	6	0	6	5666.4068	-0.0037
4	2	3	←	3	1	3	5784.0726	-0.0263
10	1	10	←	9	1	9	5844.3365	0.0045
10	0	10	←	9	0	9	5919.1955	0.0040
10	2	9	←	9	2	8	5975.3268	-0.0007
10	6	5	←	9	6	4	5991.4661	0.0007
10	5	6	←	9	5	5	5991.5579	-0.0016
10	7	3	←	9	7	2	5991.9252	0.0133
10	4	7	←	9	4	6	5992.6210	-0.0138
10	4	6	←	9	4	5	5992.6691	-0.0359
10	3	8	←	9	3	7	5994.5619	-0.0029
10	3	7	←	9	3	6	5998.1889	0.0001
10	2	8	←	9	2	7	6041.9522	-0.0016
10	1	9	←	9	1	8	6092.9488	-0.0035
8	1	7	←	7	0	7	6380.4956	-0.0170
11	1	11	←	10	1	10	6425.2322	0.0095
5	2	4	←	4	1	4	6433.2888	0.0013
11	0	11	←	10	0	10	6497.7082	0.0064
11	2	10	←	10	2	9	6569.7813	-0.0016
11	6	5	←	10	6	4	6590.7393	-0.0037
11	5	7	←	10	5	6	6591.0658	0.0020
11	4	8	←	10	4	7	6592.6359	0.0021
11	4	7	←	10	4	6	6592.7681	-0.0057
11	3	9	←	10	3	8	6594.8533	-0.0049
11	3	8	←	10	3	7	6600.7130	0.0012
11	2	9	←	10	2	8	6656.0709	-0.0007
11	1	10	←	10	1	9	6696.7288	-0.0031
12	1	12	←	11	1	11	7005.3107	0.0111
12	0	12	←	11	0	11	7073.7767	0.0086
6	2	5	←	5	1	5	7095.0847	-0.0007
9	1	8	←	8	0	8	7114.2866	-0.0106

12	2	11	←	11	2	10	7163.3774	-0.0006
12	6	7	←	11	6	6	7190.0631	0.0058
12	7	5	←	11	7	4	7190.2917	-0.0081
12	5	8	←	11	5	7	7190.6679	0.0015
12	4	9	←	11	4	8	7192.8239	-0.0029
12	4	8	←	11	4	7	7193.0866	-0.0020
12	3	10	←	11	3	9	7195.1923	-0.0034
12	3	9	←	11	3	8	7204.2184	-0.0121
12	2	10	←	11	2	9	7271.6220	-0.0001
7	2	5	←	6	1	5	7293.4242	0.0102
12	1	11	←	11	1	10	7298.7126	-0.0024
13	1	13	←	12	1	12	7584.5798	0.0137
13	0	13	←	12	0	12	7647.7953	0.0129
13	2	12	←	12	2	11	7756.0529	0.0066
7	2	6	←	6	1	6	7769.5477	0.0067
13	6	8	←	12	6	7	7789.4048	-0.0067
13	5	9	←	12	5	8	7790.3770	0.0011
13	4	10	←	12	4	9	7793.2178	-0.0031
13	4	9	←	12	4	8	7793.6839	-0.0003
13	3	11	←	12	3	10	7795.5044	-0.0011
13	3	10	←	12	3	9	7808.9268	0.0031
8	2	6	←	7	1	6	7839.7377	0.0088
10	1	9	←	9	0	9	7869.3175	0.0176
13	2	11	←	12	2	10	7888.1095	-0.0004
13	1	12	←	12	1	11	7898.6475	-0.0031
							RMS	**8.25 kHz**

Table S14. List of assigned transitions for phenol dimer, $^{13}C(4)$ isotopologue.

J'	K_a '	K_c '	←	J''	K_a''	K_c ''	ν_{obs} (MHz)	ν_{obs} - ν_{calc}
4	1	4	←	3	1	3	2332.9216	-0.0026
2	1	1	←	1	0	1	2338.0972	0.0082
4	0	4	←	3	0	3	2379.9863	0.0179
4	2	3	←	3	2	2	2384.0725	0.0012
4	2	2	←	3	2	1	2388.3951	0.0099
7	0	7	←	6	1	5	2751.5570	0.0036
5	1	5	←	4	1	4	2915.3237	0.0034
5	0	5	←	4	0	4	2971.6856	0.0018
3	1	2	←	2	0	2	2972.2455	-0.0021
5	2	4	←	4	2	3	2979.4846	0.0011
5	3	3	←	4	3	2	2982.0616	-0.0127
5	2	3	←	4	2	2	2988.0862	0.0005
5	1	4	←	4	1	3	3041.5501	-0.0007
6	2	5	←	6	1	5	3062.3846	-0.0095
5	2	4	←	5	1	4	3136.3972	0.0055
4	2	3	←	4	1	3	3198.4612	0.0021
8	0	8	←	7	1	6	3229.6737	-0.0053
3	2	2	←	3	1	2	3248.3657	0.0032
4	2	2	←	4	1	4	3457.6267	0.0027
5	2	3	←	5	1	5	3530.3918	0.0025
6	0	6	←	5	0	5	3561.2692	0.0010
6	2	5	←	5	2	4	3574.4927	0.0001
6	4	3	←	5	4	2	3578.4648	0.0034
6	3	4	←	5	3	3	3578.9190	0.0034
6	3	3	←	5	3	2	3579.1762	0.0025
6	2	4	←	5	2	3	3589.4699	0.0010
4	1	3	←	3	0	3	3619.7049	-0.0028
6	2	4	←	6	1	6	3622.6743	0.0015
6	1	5	←	5	1	4	3648.4902	0.0000
7	1	7	←	6	1	6	4078.4395	0.0015
7	0	7	←	6	0	6	4148.3838	0.0023
7	2	6	←	6	2	5	4169.0200	0.0010
7	5	2	←	6	5	1	4175.0458	-0.0007
7	4	4	←	6	4	3	4175.1744	0.0017
7	3	5	←	6	3	4	4175.9479	-0.0008
7	3	4	←	6	3	3	4176.5264	-0.0020
7	2	5	←	6	2	4	4192.7864	0.0013
7	1	6	←	6	1	5	4254.6391	-0.0012
5	1	4	←	4	0	4	4281.2961	0.0061
2	2	0	←	1	1	0	4503.8268	-0.0018
2	2	1	←	1	1	1	4528.6766	0.0039

8	1	8	←	7	1	7	4659.0098	0.0005
8	0	8	←	7	0	7	4732.7652	-0.0007
8	2	7	←	7	2	6	4762.9848	0.0004
8	5	4	←	7	5	3	4771.6659	0.0014
8	4	5	←	7	4	4	4772.0281	0.0074
8	3	6	←	7	3	5	4773.1330	-0.0396
8	3	5	←	7	3	4	4774.3288	-0.0003
8	2	6	←	7	2	5	4798.1991	-0.0027
8	1	7	←	7	1	6	4859.8342	-0.0007
6	1	5	←	5	0	5	4958.0783	-0.0181
3	2	1	←	2	1	1	5076.4314	0.0055
3	2	2	←	2	1	2	5150.0992	0.0074
9	1	9	←	8	1	8	5238.8475	0.0031
9	0	9	←	8	0	8	5314.2781	0.0007
9	2	8	←	8	2	7	5356.3131	0.0022
9	5	5	←	8	5	4	5368.3545	-0.0008
9	6	3	←	8	6	2	5368.4278	-0.0091
9	7	2	←	8	7	1	5368.9386	-0.0003
9	4	5	←	8	4	4	5369.0629	0.0076
9	3	7	←	8	3	6	5370.5721	-0.0008
9	3	6	←	8	3	5	5372.6865	0.0007
9	2	7	←	8	2	6	5405.7710	-0.0005
9	3	7	←	9	2	7	5440.8541	0.0108
9	1	8	←	8	1	7	5463.8910	-0.0008
8	3	6	←	8	2	6	5476.0390	-0.0028
5	3	3	←	5	2	3	5528.4675	0.0068
4	3	2	←	4	2	2	5534.4404	-0.0316
4	3	1	←	4	2	3	5540.9851	0.0063
6	3	3	←	6	2	5	5548.3512	0.0036
7	3	4	←	7	2	6	5555.8602	0.0033
8	3	5	←	8	2	7	5567.2093	0.0076
4	2	2	←	3	1	2	5638.9139	0.0056
7	1	6	←	6	0	6	5651.4680	-0.0005
4	2	3	←	3	1	3	5784.0726	-0.0012
10	1	10	←	9	1	9	5817.9054	0.0021
10	0	10	←	9	0	9	5892.9120	-0.0001
10	2	9	←	9	2	8	5948.9239	0.0006
10	6	5	←	9	6	4	5965.0421	0.0024
10	5	6	←	9	5	5	5965.1284	0.0008
10	4	7	←	9	4	6	5966.1976	0.0024
10	3	8	←	9	3	7	5968.1209	0.0005
10	3	7	←	9	3	6	5971.7248	-0.0012
10	2	8	←	9	2	7	6015.4044	-0.0008
10	1	9	←	9	1	8	6066.6108	-0.0006
5	2	3	←	4	1	3	6193.0195	0.0003
8	1	7	←	7	0	7	6362.9210	-0.0008

11	1	11	←	10	1	10	6396.1620	0.0012
5	2	4	←	4	1	4	6430.6327	-0.0003
11	0	11	←	10	0	10	6468.8142	-0.0017
11	2	10	←	10	2	9	6540.7492	0.0013
11	6	5	←	10	6	4	6561.6814	0.0046
11	5	7	←	10	5	6	6562.0240	0.0339
11	4	8	←	10	4	7	6563.5526	0.0017
11	4	7	←	10	4	6	6563.6899	0.0000
11	3	9	←	10	3	8	6565.7717	0.0001
11	3	8	←	10	3	7	6571.5962	0.0006
11	2	9	←	10	2	8	6626.8599	-0.0016
11	1	10	←	10	1	9	6667.7771	0.0010
6	2	4	←	5	1	4	6740.9404	0.0032
12	1	12	←	11	1	11	6973.6101	0.0037
12	0	12	←	11	0	11	7042.2747	0.0008
6	2	5	←	5	1	5	7089.8048	-0.0004
9	1	8	←	8	0	8	7094.0443	-0.0033
12	2	11	←	11	2	10	7131.7159	0.0011
12	6	6	←	11	6	5	7158.3488	-0.0025
12	5	8	←	11	5	7	7158.9486	-0.0030
12	4	9	←	11	4	8	7161.0961	-0.0049
12	3	10	←	11	3	9	7163.4694	0.0009
12	3	9	←	11	3	8	7172.4576	-0.0004
12	2	10	←	11	2	9	7239.7532	-0.0036
12	1	11	←	11	1	10	7267.1505	-0.0004
7	2	5	←	6	1	5	7285.2330	0.0008
13	1	13	←	12	1	12	7550.2472	0.0038
13	0	13	←	12	0	12	7613.6791	0.0034
13	2	12	←	12	2	11	7721.7606	0.0029
13	6	7	←	12	6	6	7755.0659	-0.0004
13	7	6	←	12	7	5	7755.1512	-0.0063
13	4	10	←	12	4	9	7758.8537	0.0014
13	4	9	←	12	4	8	7759.2923	-0.0200
13	3	11	←	12	3	10	7761.1402	0.0006
7	2	6	←	6	1	6	7761.6029	-0.0360
13	3	10	←	12	3	9	7774.4911	-0.0002
8	2	6	←	7	1	6	7828.7919	-0.0017
10	1	9	←	9	0	9	7846.4060	0.0243
13	2	11	←	12	2	10	7853.5953	-0.0029
13	1	12	←	12	1	11	7864.4852	-0.0003
4	3	1	←	3	2	1	7922.8925	0.0029
4	3	2	←	3	2	2	7925.0122	-0.0056
							RMS	**7.98 kHz**

Table S15. List of assigned transitions for phenol dimer, $^{13}C(5)$ isotopologue.

J'	K_a '	K_c '	←	J''	K_a''	K_c ''	ν_{obs} (MHz)	ν_{obs} - ν_{calc}
6	0	6	←	5	1	4	2242.1093	0.0006
4	1	4	←	3	1	3	2330.0023	-0.0535
2	1	1	←	1	0	1	2343.5122	-0.0119
4	0	4	←	3	0	3	2376.4945	0.0005
4	2	3	←	3	2	2	2380.4474	-0.0081
4	2	2	←	3	2	1	2384.6161	-0.0008
4	1	3	←	3	1	2	2429.6538	0.0038
8	2	7	←	8	1	7	2909.4753	-0.0100
5	1	5	←	4	1	4	2911.7633	0.0006
5	0	5	←	4	0	4	2967.4549	0.0006
5	2	4	←	4	2	3	2974.9831	-0.0006
5	4	2	←	4	4	1	2977.3134	0.0152
5	2	3	←	4	2	2	2983.2834	0.0005
5	1	4	←	4	1	3	3036.1764	-0.0002
5	2	4	←	5	1	4	3162.4491	0.0036
4	2	3	←	4	1	3	3223.6504	0.0121
3	2	2	←	3	1	2	3272.8322	-0.0007
3	2	1	←	3	1	3	3424.3662	-0.0038
4	2	2	←	4	1	4	3478.9301	-0.0010
6	1	6	←	5	1	5	3492.9564	0.0009
5	2	3	←	5	1	5	3550.4476	-0.0038
6	0	6	←	5	0	5	3556.3554	0.0000
6	2	5	←	5	2	4	3569.1233	0.0010
6	4	3	←	5	4	2	3572.9698	0.0026
6	3	4	←	5	3	3	3573.3991	0.0008
6	3	3	←	5	3	2	3573.6446	0.0027
6	2	4	←	5	2	3	3583.5737	-0.0002
4	1	3	←	3	0	3	3622.0175	-0.0009
6	1	5	←	5	1	4	3642.0889	0.0001
7	1	7	←	6	1	6	4073.5569	0.0019
7	0	7	←	6	0	6	4142.8651	-0.0003
7	2	6	←	6	2	5	4162.7957	0.0014
7	5	2	←	6	5	1	4168.6396	-0.0025
7	4	4	←	6	4	3	4168.7483	-0.0011
7	3	5	←	6	3	4	4169.4910	-0.0014
7	3	4	←	6	3	3	4170.0413	0.0016
7	2	5	←	6	2	4	4185.7358	0.0009
7	1	6	←	6	1	5	4247.2391	-0.0012
5	1	4	←	4	0	4	4281.6989	-0.0021
2	2	0	←	1	1	0	4525.5665	-0.0020
2	2	1	←	1	1	1	4550.0645	0.0012

8	1	8	←	7	1	7	4653.4928	-0.0012
8	0	8	←	7	0	7	4726.7282	-0.0005
8	2	7	←	7	2	6	4755.9242	0.0007
8	5	4	←	7	5	3	4764.3303	-0.0048
8	6	2	←	7	6	1	4764.5360	-0.0125
8	4	5	←	7	4	4	4764.6676	0.0052
8	7	1	←	7	7	0	4765.0709	-0.0049
8	3	6	←	7	3	5	4765.7725	0.0008
8	3	5	←	7	3	4	4766.8628	-0.0009
8	2	6	←	7	2	5	4789.9585	0.0246
8	1	7	←	7	1	6	4851.4710	-0.0003
6	1	5	←	5	0	5	4956.3281	-0.0075
3	2	1	←	2	1	1	5097.5626	0.0007
3	2	2	←	2	1	2	5170.2124	0.0018
9	1	9	←	8	1	8	5232.7201	0.0019
9	0	9	←	8	0	8	5307.7972	0.0004
9	2	8	←	8	2	7	5348.4357	0.0007
9	5	5	←	8	5	4	5360.0989	0.0022
9	6	3	←	8	6	2	5360.1969	-0.0013
9	4	5	←	8	4	4	5360.7627	0.0101
9	3	7	←	8	3	6	5362.2225	-0.0007
9	3	6	←	8	3	5	5364.2166	-0.0020
9	2	7	←	8	2	6	5396.2296	-0.0016
10	3	8	←	10	2	8	5437.5021	-0.0061
9	1	8	←	8	1	7	5454.6061	-0.0011
9	3	7	←	9	2	7	5483.2499	0.0076
8	3	6	←	8	2	6	5517.2486	-0.0016
6	3	4	←	6	2	4	5557.6503	-0.0046
5	3	2	←	5	2	4	5582.4779	-0.0192
6	3	3	←	6	2	5	5587.0249	0.0081
7	3	4	←	7	2	6	5594.2778	0.0156
8	3	5	←	8	2	7	5605.2017	-0.0007
7	1	6	←	6	0	6	5647.2189	-0.0015
4	2	2	←	3	1	2	5659.5338	-0.0001
4	2	3	←	3	1	3	5802.7163	-0.0251
10	1	10	←	9	1	9	5811.1883	0.0009
10	0	10	←	9	0	9	5886.0521	-0.0002
10	2	9	←	9	2	8	5940.2565	0.0010
10	5	6	←	9	5	5	5955.9346	-0.0010
10	4	6	←	9	4	5	5957.0080	-0.0023
10	4	7	←	9	4	6	5956.9538	0.0079
10	3	8	←	9	3	7	5958.8193	-0.0007
10	3	7	←	9	3	6	5962.2239	-0.0015
10	2	8	←	9	2	7	6004.5518	-0.0023
10	1	9	←	9	1	8	6056.4648	0.0078
5	2	3	←	4	1	3	6213.1703	0.0036

8	1	7	←	7	0	7	6355.8234	-0.0028
11	1	11	←	10	1	10	6388.8748	-0.0010
5	2	4	←	4	1	4	6447.6699	0.0005
11	0	11	←	10	0	10	6461.6225	0.0007
11	2	10	←	10	2	9	6531.3140	0.0001
11	5	7	←	10	5	6	6551.8607	0.0012
11	7	4	←	10	7	3	6551.9725	-0.0018
11	4	8	←	10	4	7	6553.3447	-0.0001
11	4	7	←	10	4	6	6553.4728	-0.0004
11	3	9	←	10	3	8	6555.5222	0.0010
11	3	8	←	10	3	7	6561.0236	0.0006
11	2	9	←	10	2	8	6614.6828	-0.0013
11	1	10	←	10	1	9	6656.8133	0.0009
6	2	4	←	5	1	4	6760.5623	-0.0017
12	1	12	←	11	1	11	6965.7729	0.0013
12	0	12	←	11	0	11	7034.7675	0.0012
6	2	5	←	5	1	5	7105.0290	-0.0001
12	2	11	←	11	2	10	7121.5430	0.0009
12	6	6	←	11	6	5	7147.3218	-0.0063
12	7	5	←	11	7	4	7147.5983	-0.0070
12	5	8	←	11	5	7	7147.8774	0.0005
12	8	4	←	11	8	3	7148.4382	0.0379
12	9	3	←	11	9	2	7149.5516	-0.0187
12	4	9	←	11	4	8	7149.9298	0.0000
12	4	8	←	11	4	7	7150.1694	-0.0005
12	3	10	←	11	3	9	7152.2715	-0.0005
12	3	9	←	11	3	8	7160.7656	-0.0012
12	1	11	←	11	1	10	7255.4493	0.0010
7	2	5	←	6	1	5	7304.2119	0.0018
13	1	13	←	12	1	12	7541.8756	-0.0008
13	0	13	←	12	0	12	7605.8486	-0.0031
16	4	13	←	16	3	13	7680.1701	-0.0026
13	2	12	←	12	2	11	7710.8778	0.0024
13	6	7	←	12	6	6	7743.1084	0.0003
13	5	9	←	12	5	8	7744.0011	0.0056
13	4	10	←	12	4	9	7746.7092	0.0009
13	4	9	←	12	4	8	7747.1348	0.0013
13	3	11	←	12	3	10	7749.0049	-0.0002
13	3	10	←	12	3	9	7761.6029	-0.0242
7	2	6	←	6	1	6	7774.9030	0.0352
10	1	9	←	9	0	9	7832.3548	-0.0102
13	2	11	←	12	2	10	7838.8332	0.0011
8	2	6	←	7	1	6	7846.9009	-0.0029
13	1	12	←	12	1	11	7852.1283	0.0034
4	3	2	←	3	2	2	7960.3296	0.0048

4	3	1	←	3	2	1	7958.2730	0.0016
							RMS	**8.75 kHz**

Table S16. List of assigned transitions for phenol dimer, $^{13}C(6)$ isotopologue.

J'	K_a '	K_c '	←	J''	K_a''	K_c ''	ν_{obs} (MHz)	ν_{obs} - ν_{calc}
4	1	4	←	3	1	3	2337.8352	0.0043
4	0	4	←	3	0	3	2384.4025	-0.0002
4	2	3	←	3	2	2	2388.3951	-0.0020
4	2	2	←	3	2	1	2392.5907	-0.0046
8	2	7	←	8	1	7	2900.5448	-0.0162
5	1	5	←	4	1	4	2921.4739	-0.0009
5	0	5	←	4	0	4	2977.3134	0.0005
3	1	2	←	2	0	2	2979.9132	-0.0009
5	2	4	←	4	2	3	2984.8826	-0.0233
5	3	3	←	4	3	2	2987.4178	-0.0127
5	3	2	←	4	3	1	2987.5238	0.0005
5	2	3	←	4	2	2	2993.2793	0.0013
7	2	6	←	7	1	6	2996.3974	-0.0019
5	1	4	←	4	1	3	3046.2950	0.0004
6	2	5	←	6	1	5	3081.0970	-0.0111
6	1	6	←	5	1	5	3504.6006	0.0001
6	0	6	←	5	0	5	3568.1479	0.0013
6	2	5	←	5	2	4	3581.0220	0.0005
6	4	3	←	5	4	2	3584.8952	0.0035
6	3	4	←	5	3	3	3585.3294	-0.0016
6	3	3	←	5	3	2	3585.5782	0.0000
6	2	4	←	5	2	3	3595.5995	-0.0002
4	1	3	←	3	0	3	3627.8629	-0.0022
6	1	5	←	5	1	4	3654.2194	0.0005
7	1	7	←	6	1	6	4087.1287	0.0004
7	0	7	←	6	0	6	4156.5702	0.0003
7	2	6	←	6	2	5	4176.6669	0.0001
7	5	3	←	6	5	2	4182.5466	-0.0016
7	4	4	←	6	4	3	4182.6635	-0.0009
7	3	5	←	6	3	4	4183.4173	-0.0013
7	3	4	←	6	3	3	4183.9718	-0.0019
7	2	5	←	6	2	4	4199.8066	0.0002
7	1	6	←	6	1	5	4261.3751	-0.0005
5	1	4	←	4	0	4	4289.7333	-0.0238
2	2	1	←	1	1	1	4546.5291	-0.0050
8	1	8	←	7	1	7	4668.9890	-0.0014
8	0	8	←	7	0	7	4742.3273	0.0005
8	2	7	←	7	2	6	4771.7644	-0.0004
8	5	3	←	7	5	2	4780.2252	-0.0050

8	4	5	←	7	4	4	4780.5750	0.0057
8	7	1	←	7	7	0	4780.9941	0.0406
8	3	6	←	7	3	5	4781.6931	0.0006
8	3	5	←	7	3	4	4782.7988	-0.0015
8	2	6	←	7	2	5	4806.0633	-0.0029
8	1	7	←	7	1	6	4867.6013	-0.0019
6	1	5	←	5	0	5	4966.6685	0.0054
3	2	2	←	2	1	2	5168.7502	0.0014
9	1	9	←	8	1	8	5250.1327	0.0002
9	0	9	←	8	0	8	5325.2701	0.0003
9	2	8	←	8	2	7	5366.2384	-0.0016
9	5	5	←	8	5	4	5377.9792	-0.0025
9	6	3	←	8	6	2	5378.0720	0.0003
9	4	5	←	8	4	4	5378.6774	0.0238
9	3	7	←	8	3	6	5380.1405	0.0010
9	3	6	←	8	3	5	5382.1608	-0.0028
9	2	7	←	8	2	6	5414.4341	-0.0030
9	1	8	←	8	1	7	5472.7248	-0.0008
4	2	2	←	3	1	2	5659.7476	0.0021
4	2	3	←	3	1	3	5803.3901	0.0035
10	1	10	←	9	1	9	5830.5140	-0.0007
10	0	10	←	9	0	9	5905.3846	-0.0004
10	2	9	←	9	2	8	5960.0210	0.0027
10	5	6	←	9	5	5	5975.8123	0.0010
10	4	7	←	9	4	6	5976.8416	0.0002
10	4	6	←	9	4	5	5976.8900	-0.0171
10	3	8	←	9	3	7	5978.7345	0.0024
10	3	7	←	9	3	6	5982.1845	-0.0021
10	2	8	←	9	2	7	6024.8400	-0.0027
10	1	9	←	9	1	8	6076.5495	0.0002
5	2	3	←	4	1	3	6215.2747	0.0018
8	1	7	←	7	0	7	6370.9134	-0.0120
11	1	11	←	10	1	10	6410.1122	0.0012
5	2	4	←	4	1	4	6450.4648	0.0033
11	0	11	←	10	0	10	6482.8024	-0.0011
11	2	10	←	10	2	9	6553.0321	0.0037
11	6	5	←	10	6	4	6573.4307	-0.0045
11	5	7	←	10	5	6	6573.7220	-0.0052
11	4	8	←	10	4	7	6575.2360	-0.0013
11	4	7	←	10	4	6	6575.3670	-0.0013
11	3	9	←	10	3	8	6577.4271	-0.0017
11	3	8	←	10	3	7	6583.0086	-0.0011
11	2	9	←	10	2	8	6637.0581	-0.0007
11	1	10	←	10	1	9	6678.8648	0.0009
6	2	4	←	5	1	4	6764.5810	0.0031
12	1	12	←	11	1	11	6988.9100	0.0001

12	0	12	←	11	0	11	7057.7927	0.0001
9	1	8	←	8	0	8	7101.3288	0.0047
6	2	5	←	5	1	5	7110.0114	0.0031
12	2	11	←	11	2	10	7145.2047	0.0034
12	6	7	←	11	6	6	7171.1635	-0.0043
12	5	8	←	11	5	7	7171.7374	-0.0005
12	4	9	←	11	4	8	7173.8212	0.0000
12	4	8	←	11	4	7	7174.0657	-0.0004
12	3	10	←	11	3	9	7176.1755	0.0014
12	3	9	←	11	3	8	7184.7884	-0.0018
12	2	10	←	11	2	9	7250.7199	-0.0025
12	1	11	←	11	1	10	7279.4455	0.0038
7	2	5	←	6	1	5	7310.1644	-0.0010
13	1	13	←	12	1	12	7566.9136	-0.0001
13	0	13	←	12	0	12	7630.7243	0.0005
13	2	12	←	12	2	11	7736.4789	0.0066
13	4	10	←	13	3	10	7743.1084	-0.0094
13	6	8	←	12	6	7	7768.9315	-0.0065
13	7	6	←	12	7	5	7769.0448	0.0000
13	5	9	←	12	5	8	7769.8536	0.0025
13	4	9	←	12	4	8	7773.0325	-0.0016
13	3	11	←	12	3	10	7774.9030	0.0036
13	3	10	←	12	3	9	7787.6995	-0.0009
10	1	9	←	9	0	9	7852.5992	-0.0045
13	2	11	←	12	2	10	7865.3605	-0.0013
13	1	12	←	12	1	11	7878.0445	0.0039
4	3	1	←	3	2	1	7953.6423	0.0096
4	3	2	←	3	2	2	7955.7244	0.0202
							RMS	**6.98 kHz**

Table S17. List of assigned transitions for phenol dimer, $^{13}C(9)$ isotopologue.

J'	K_a '	K_c '	←	J''	K_a''	K_c ''	ν_{obs} (MHz)	ν_{obs} - ν_{calc}
4	1	4	←	3	1	3	2347.0355	0.0008
2	1	1	←	1	0	1	2350.7041	-0.0311
4	0	4	←	3	0	3	2394.2119	-0.0035
4	2	3	←	3	2	2	2398.3257	0.0047
4	2	2	←	3	2	1	2402.6380	0.0007
4	1	3	←	3	1	2	2448.3588	-0.0037
7	0	7	←	6	1	5	2770.3137	0.0007
8	2	7	←	8	1	7	2894.9284	-0.0041
5	1	5	←	4	1	4	2932.9586	0.0007
3	1	2	←	2	0	2	2988.5579	-0.0024
5	0	5	←	4	0	4	2989.4900	-0.0005
7	2	6	←	7	1	6	2992.0514	-0.0067
5	2	4	←	4	2	3	2997.2959	0.0006
5	4	2	←	4	4	1	2999.6933	0.0115
5	2	3	←	4	2	2	3005.9029	0.0006
5	1	4	←	4	1	3	3059.5364	0.0013
6	2	5	←	6	1	5	3077.9159	-0.0042
5	2	4	←	5	1	4	3152.1250	0.0006
4	2	3	←	4	1	3	3214.3646	0.0002
3	2	2	←	3	1	2	3264.4104	0.0045
2	2	0	←	2	1	2	3378.5455	0.0025
3	2	1	←	3	1	3	3418.6288	0.0054
4	2	2	←	4	1	4	3474.2233	-0.0028
6	1	6	←	5	1	5	3518.3494	0.0000
5	2	3	←	5	1	5	3547.1765	0.0060
6	0	6	←	5	0	5	3582.6334	0.0005
6	2	5	←	5	2	4	3595.8679	0.0016
6	4	3	←	5	4	2	3599.8343	-0.0029
6	3	4	←	5	3	3	3600.2944	0.0025
6	3	3	←	5	3	2	3600.5458	-0.0038
6	2	4	←	5	2	3	3610.8508	-0.0005
4	1	3	←	3	0	3	3639.7394	0.0174
6	1	5	←	5	1	4	3670.0714	0.0007
7	2	5	←	7	1	7	3754.2850	0.0053
7	1	7	←	6	1	6	4103.1290	0.0011
10	0	10	←	9	1	8	4141.6501	0.0051
7	0	7	←	6	0	6	4173.3024	0.0004
7	2	6	←	6	2	5	4193.9546	0.0001
7	5	2	←	6	5	1	4199.9761	-0.0091
7	4	4	←	6	4	3	4200.1143	0.0030

7	3	5	←	6	3	4	4200.8898	0.0015
7	3	4	←	6	3	3	4201.4664	-0.0006
7	2	5	←	6	2	4	4217.7347	-0.0005
7	1	6	←	6	1	5	4279.8098	-0.0069
5	1	4	←	4	0	4	4305.0281	-0.0135
2	2	0	←	1	1	0	4527.1867	0.0165
2	2	1	←	1	1	1	4552.0787	-0.0047
8	1	8	←	7	1	7	4687.2246	0.0002
8	0	8	←	7	0	7	4761.2388	-0.0002
8	2	7	←	7	2	6	4791.4801	-0.0011
8	5	3	←	7	5	2	4800.1632	-0.0027
8	6	2	←	7	6	1	4800.3675	0.0009
8	4	5	←	7	4	4	4800.5293	0.0071
8	3	6	←	7	3	5	4801.6759	-0.0001
8	3	5	←	7	3	4	4802.8320	0.0016
8	2	6	←	7	2	5	4826.7228	0.0008
8	1	7	←	7	1	6	4888.6068	0.0000
6	1	5	←	5	0	5	4985.6244	0.0026
3	2	1	←	2	1	1	5103.2604	-0.0012
3	2	2	←	2	1	2	5177.1346	0.0003
9	1	9	←	8	1	8	5270.5844	0.0005
13	0	13	←	12	1	11	5274.0703	-0.0033
9	0	9	←	8	0	8	5346.2989	-0.0002
9	2	8	←	8	2	7	5388.3674	-0.0015
9	5	5	←	8	5	4	5400.4156	-0.0038
9	6	3	←	8	6	2	5400.4972	-0.0039
9	4	5	←	8	4	4	5401.1275	0.0081
9	3	7	←	8	3	6	5402.6408	0.0005
9	3	6	←	8	3	5	5404.7507	0.0012
9	2	7	←	8	2	6	5437.8664	0.0010
9	1	8	←	8	1	7	5496.2582	-0.0008
8	3	6	←	8	2	6	5503.0725	-0.0119
7	3	5	←	7	2	5	5528.1295	-0.0009
6	3	4	←	6	2	4	5544.9838	0.0065
5	3	3	←	5	2	3	5555.5360	-0.0007
3	3	0	←	3	2	2	5566.6931	0.0017
4	3	1	←	4	2	3	5568.0596	-0.0020
5	3	2	←	5	2	4	5570.7486	-0.0020
6	3	3	←	6	2	5	5575.4406	0.0067
7	3	4	←	7	2	6	5582.9574	0.0111
8	3	5	←	8	2	7	5594.2778	-0.0177
9	3	6	←	9	2	8	5610.6870	0.0108
4	2	2	←	3	1	2	5669.2067	0.0019
7	1	6	←	6	0	6	5682.8038	-0.0018
13	3	10	←	13	2	12	5757.8378	-0.0055
4	2	3	←	3	1	3	5814.7849	0.0021

10	1	10	←	9	1	9	5853.1658	-0.0003
10	0	10	←	9	0	9	5928.4762	-0.0002
10	2	9	←	9	2	8	5984.5392	-0.0025
10	6	4	←	9	6	3	6000.6689	0.0022
10	5	6	←	9	5	5	6000.7590	0.0047
10	4	7	←	9	4	6	6001.8214	-0.0012
10	4	6	←	9	4	5	6001.8950	0.0031
10	3	8	←	9	3	7	6003.7500	-0.0027
10	3	7	←	9	3	6	6007.3499	-0.0021
10	2	8	←	9	2	7	6051.0788	0.0009
10	1	9	←	9	1	8	6102.5723	-0.0015
5	2	3	←	4	1	3	6226.7474	0.0029
8	1	7	←	7	0	7	6398.1107	0.0004
11	1	11	←	10	1	10	6434.9468	0.0013
5	2	4	←	4	1	4	6465.0399	-0.0035
11	0	11	←	10	0	10	6507.9156	-0.0003
11	2	10	←	10	2	9	6579.9251	-0.0016
11	6	5	←	10	6	4	6600.8653	-0.0011
11	5	7	←	10	5	6	6601.1916	0.0120
11	4	8	←	10	4	7	6602.7419	0.0005
11	4	7	←	10	4	6	6602.8779	-0.0019
11	3	9	←	10	3	8	6604.9660	-0.0034
11	3	8	←	10	3	7	6610.7835	0.0000
11	2	9	←	10	2	8	6666.1202	0.0009
11	1	10	←	10	1	9	6707.3302	-0.0033
6	2	4	←	5	1	4	6778.0602	-0.0005
12	1	12	←	11	1	11	7015.9114	-0.0001
12	0	12	←	11	0	11	7084.9035	0.0021
6	2	5	←	5	1	5	7127.9510	-0.0008
9	1	8	←	8	0	8	7133.1223	-0.0081
12	2	11	←	11	2	10	7174.4497	-0.0034
12	6	6	←	11	6	5	7201.0996	-0.0038
12	7	5	←	11	7	4	7201.3544	0.0002
12	5	8	←	11	5	7	7201.7096	0.0058
12	4	9	←	11	4	8	7203.8539	-0.0009
12	4	8	←	11	4	7	7204.1158	0.0023
12	3	10	←	11	3	9	7206.2318	-0.0010
							RMS	**5.53 kHz**

Table S18. List of assigned transitions for phenol dimer, ^{13}C(10) isotopologue.

J'	K_a '	K_c '	←	J''	K_a''	K_c ''	ν_{obs} (MHz)	ν_{obs} - ν_{calc}
4	1	4	←	3	1	3	2349.7229	0.0048
2	1	1	←	1	0	1	2350.4231	-0.0020
11	1	11	←	10	2	9	2396.6441	0.0003
4	2	3	←	3	2	2	2400.7102	0.0010
4	3	2	←	3	3	1	2402.0365	-0.0038
4	1	3	←	3	1	2	2450.4672	0.0009
5	1	5	←	4	1	4	2936.3190	-0.0008
3	1	2	←	2	0	2	2988.6044	-0.0228
5	0	5	←	4	0	4	2992.5584	-0.0008
5	2	4	←	4	2	3	3000.2848	-0.0011
5	3	2	←	4	3	1	3002.9371	-0.0129
5	2	3	←	4	2	2	3008.8046	-0.0010
5	1	4	←	4	1	3	3062.1733	-0.0003
6	2	5	←	6	1	5	3075.5461	-0.0051
5	2	4	←	5	1	4	3149.3397	0.0013
4	2	3	←	4	1	3	3211.2514	0.0253
3	2	2	←	3	1	2	3260.9846	0.0013
2	2	0	←	2	1	2	3374.4605	-0.0057
3	2	1	←	3	1	3	3414.3131	0.0042
4	2	2	←	4	1	4	3469.5729	0.0005
6	1	6	←	5	1	5	3522.3939	-0.0008
5	2	3	←	5	1	5	3542.0656	0.0074
6	0	6	←	5	0	5	3586.3606	-0.0017
6	2	5	←	5	2	4	3599.4620	-0.0008
6	4	3	←	5	4	2	3603.4060	0.0051
6	3	4	←	5	3	3	3603.8473	0.0002
6	3	3	←	5	3	2	3604.1020	0.0009
6	2	4	←	5	2	3	3614.2954	-0.0010
6	2	4	←	6	1	6	3633.9618	0.0018
4	1	3	←	3	0	3	3640.0849	-0.0016
6	1	5	←	5	1	4	3673.2486	-0.0015
7	2	5	←	7	1	7	3747.8106	0.0095
7	1	7	←	6	1	6	4107.8614	-0.0005
7	0	7	←	6	0	6	4177.7139	-0.0015
7	2	6	←	6	2	5	4198.1604	-0.0008
7	5	2	←	6	5	1	4204.1386	-0.0071
7	4	4	←	6	4	3	4204.2653	0.0011
7	3	5	←	6	3	4	4205.0302	0.0007
7	2	5	←	6	2	4	4221.7002	-0.0029
7	1	6	←	6	1	5	4283.5437	-0.0010

5	1	4	←	4	0	4	4305.6169	0.0011
2	2	1	←	1	1	1	4549.3504	0.0021
8	1	8	←	7	1	7	4692.6510	-0.0020
8	0	8	←	7	0	7	4766.3590	-0.0019
8	2	7	←	7	2	6	4796.3005	-0.0024
8	4	4	←	7	4	3	4805.2948	0.0194
8	3	6	←	7	3	5	4806.3989	-0.0019
8	3	5	←	7	3	4	4807.5369	-0.0016
8	2	6	←	7	2	5	4831.1921	-0.0014
8	1	7	←	7	1	6	4892.8932	0.0000
6	1	5	←	5	0	5	4986.3064	-0.0003
3	2	1	←	2	1	1	5101.3885	-0.0024
3	2	2	←	2	1	2	5174.8518	0.0013
9	1	9	←	8	1	8	5276.7118	-0.0013
9	0	9	←	8	0	8	5352.1517	-0.0014
9	2	8	←	8	2	7	5393.8116	0.0004
9	5	5	←	8	5	4	5405.7701	0.0110
9	6	3	←	8	6	2	5405.8546	0.0045
9	7	2	←	8	7	1	5406.3826	0.0233
9	4	5	←	8	4	4	5406.4540	0.0102
9	3	7	←	8	3	6	5407.9485	0.0015
9	3	6	←	8	3	5	5410.0242	-0.0016
10	3	8	←	10	2	8	5415.5667	-0.0023
14	7	7	←	15	6	9	5436.1420	0.0014
9	2	7	←	8	2	6	5442.8215	-0.0012
9	3	7	←	9	2	7	5462.4270	-0.0092
8	3	6	←	8	2	6	5497.3115	-0.0003
9	1	8	←	8	1	7	5501.1149	-0.0005
7	3	5	←	7	2	5	5522.1037	-0.0008
6	3	4	←	6	2	4	5538.7725	-0.0056
5	3	3	←	5	2	3	5549.2208	-0.0065
4	3	2	←	4	2	2	5555.1793	0.0010
5	3	2	←	5	2	4	5564.2875	0.0013
7	3	4	←	7	2	6	5576.3637	0.0007
8	3	5	←	8	2	7	5587.5961	-0.0026
9	3	6	←	9	2	8	5603.8148	0.0015
4	2	2	←	3	1	2	5668.1048	0.0003
7	1	6	←	6	0	6	5683.4875	-0.0016
4	2	3	←	3	1	3	5812.8792	0.0008
10	1	10	←	9	1	9	5860.0001	-0.0020
10	0	10	←	9	0	9	5935.0833	-0.0003
10	2	9	←	9	2	8	5990.6114	0.0005
10	6	4	←	9	6	3	6006.6005	-0.0051
10	5	6	←	9	5	5	6006.6859	0.0047
10	4	7	←	9	4	6	6007.7149	-0.0148
10	4	6	←	9	4	5	6007.7923	-0.0055

10	3	8	←	9	3	7	6009.6382	-0.0014
10	3	7	←	9	3	6	6013.1855	-0.0017
10	1	9	←	9	1	8	6108.0122	-0.0017
5	2	3	←	4	1	3	6226.4654	0.0217
8	1	7	←	7	0	7	6398.6663	-0.0006
11	1	11	←	10	1	10	6442.4935	-0.0008
5	2	4	←	4	1	4	6463.4457	-0.0006
11	0	11	←	10	0	10	6515.2920	-0.0005
11	2	10	←	10	2	9	6586.6310	0.0017
11	6	5	←	10	6	4	6607.3931	-0.0007
11	5	6	←	10	5	5	6607.7083	0.0151
11	8	3	←	10	8	2	6608.5757	-0.0140
11	4	8	←	10	4	7	6609.2279	0.0001
11	4	7	←	10	4	6	6609.3621	-0.0017
11	3	9	←	10	3	8	6611.4354	-0.0005
11	3	8	←	10	3	7	6617.1652	-0.0013
11	2	9	←	10	2	8	6672.0094	-0.0017
11	1	10	←	10	1	9	6713.3739	0.0000
6	2	4	←	5	1	4	6778.5666	0.0001
12	1	12	←	11	1	11	7024.1777	-0.0011
12	0	12	←	11	0	11	7093.0572	-0.0002
6	2	5	←	5	1	5	7126.6127	0.0234
12	2	11	←	11	2	10	7181.7974	0.0007
12	6	6	←	11	6	5	7208.2172	-0.0006
12	7	5	←	11	7	4	7208.4766	-0.0051
12	5	8	←	11	5	7	7208.8056	0.0068
12	4	9	←	11	4	8	7210.9190	0.0013
12	4	8	←	11	4	7	7211.1737	0.0022
12	3	10	←	11	3	9	7213.2785	0.0000
12	3	9	←	11	3	8	7222.1238	-0.0011
12	2	10	←	11	2	9	7288.9603	-0.0001
12	1	11	←	11	1	10	7316.9639	0.0011
3	3	0	←	2	2	0	7360.6529	0.0048
3	3	1	←	2	2	1	7361.0598	-0.0120
13	1	13	←	12	1	12	7605.0596	0.0011
13	0	13	←	12	0	12	7668.7604	-0.0007
13	2	12	←	12	2	11	7776.0639	0.0167
7	2	6	←	6	1	6	7802.3393	-0.0165
13	6	8	←	12	6	7	7809.0760	-0.0047
13	7	6	←	12	7	5	7809.1863	-0.0022
13	5	9	←	12	5	8	7810.0188	0.0078
13	4	10	←	12	4	9	7812.8091	0.0031
13	4	9	←	12	4	8	7813.2329	-0.0227
13	3	11	←	12	3	10	7815.1002	0.0028
13	3	10	←	12	3	9	7828.2373	-0.0008

8	2	6	←	7	1	6	7874.6689	0.0005
10	1	9	←	9	0	9	7889.2799	-0.0023
13	1	12	←	12	1	11	7918.5342	0.0007
4	3	2	←	3	2	2	7962.2905	-0.0091
4	3	1	←	3	2	1	7960.1911	-0.0006
							RMS	**6.84 kHz**

Table S19. List of assigned transitions for phenol dimer, ^{13}C(11) isotopologue.

J'	K_a '	K_c '	←	J''	K_a''	K_c ''	ν_{obs} (MHz)	ν_{obs} - ν_{calc}
4	1	4	←	3	1	3	2343.2905	0.0010
4	0	4	←	3	0	3	2390.1536	-0.0014
4	2	3	←	3	2	2	2394.2119	-0.0262
4	2	2	←	3	2	1	2398.5295	-0.0021
4	1	3	←	3	1	2	2443.9641	0.0144
8	2	7	←	8	1	7	2871.4712	-0.0021
5	1	5	←	4	1	4	2928.2829	0.0024
7	2	6	←	7	1	6	2967.9483	-0.0063
3	1	2	←	2	0	2	2976.2020	0.0085
5	0	5	←	4	0	4	2984.4335	0.0015
5	2	4	←	4	2	3	2992.1967	0.0022
5	2	3	←	4	2	2	3000.7565	0.0003
6	2	5	←	6	1	5	3053.2549	0.0065
5	1	4	←	4	1	3	3054.0247	0.0011
5	2	4	←	5	1	4	3126.9614	-0.0010
4	2	3	←	4	1	3	3188.7954	0.0039
3	2	2	←	3	1	2	3238.4901	-0.0130
4	2	2	←	4	1	4	3446.9352	-0.0140
6	1	6	←	5	1	5	3512.7395	-0.0031
6	0	6	←	5	0	5	3576.5884	0.0007
6	2	5	←	5	2	4	3589.7541	0.0044
6	3	4	←	5	3	3	3594.1520	0.0015
6	3	3	←	5	3	2	3594.4055	-0.0016
6	2	4	←	5	2	3	3604.6571	0.0015
6	2	4	←	6	1	6	3611.3374	-0.0005
4	1	3	←	3	0	3	3625.9970	0.0014
6	1	5	←	5	1	4	3663.4650	0.0013
7	1	7	←	6	1	6	4096.5981	0.0034
7	0	7	←	6	0	6	4166.2841	0.0008
7	2	6	←	6	2	5	4186.8246	0.0002
7	4	4	←	6	4	3	4192.9492	0.0044
7	3	5	←	6	3	4	4193.7072	-0.0126
7	3	4	←	6	3	3	4194.2977	0.0015
7	2	5	←	6	2	4	4210.4795	0.0003

7	1	6	←	6	1	5	4272.1173	-0.0010
5	1	4	←	4	0	4	4289.8634	-0.0009
2	2	0	←	1	1	0	4498.8115	0.0035
2	2	1	←	1	1	1	4523.5606	0.0043
8	1	8	←	7	1	7	4679.7701	0.0018
8	0	8	←	7	0	7	4753.2628	0.0010
8	2	7	←	7	2	6	4783.3398	-0.0005
8	5	4	←	7	5	3	4791.9670	-0.0042
8	6	2	←	7	6	1	4792.1699	0.0035
8	4	5	←	7	4	4	4792.3391	0.0098
8	3	6	←	7	3	5	4793.4799	0.0010
8	3	5	←	7	3	4	4794.6336	0.0048
8	2	6	←	7	2	5	4818.3939	0.0003
8	1	7	←	7	1	6	4879.8207	-0.0009
6	1	5	←	5	0	5	4968.8920	-0.0040
3	2	1	←	2	1	1	5074.0366	0.0010
3	2	2	←	2	1	2	5147.4154	-0.0031
9	1	9	←	8	1	8	5262.2090	0.0004
9	0	9	←	8	0	8	5337.3797	0.0001
9	2	8	←	8	2	7	5379.2192	-0.0011
9	5	5	←	8	5	4	5391.1953	-0.0031
9	4	5	←	8	4	4	5391.9120	0.0131
9	3	7	←	8	3	6	5393.4135	0.0000
9	3	6	←	8	3	5	5395.5140	-0.0005
9	2	7	←	8	2	6	5428.4491	-0.0025
8	3	6	←	8	2	6	5459.4209	-0.0030
7	3	5	←	7	2	5	5484.3343	-0.0043
9	1	8	←	8	1	7	5486.3911	-0.0015
6	3	4	←	6	2	4	5501.1152	0.0172
7	3	4	←	7	2	6	5538.8649	-0.0015
8	3	5	←	8	2	7	5550.1511	-0.0039
10	3	7	←	10	2	9	5589.1417	0.0017
4	2	2	←	3	1	2	5639.1894	0.0044
7	1	6	←	6	0	6	5664.4275	0.0010
4	2	3	←	3	1	3	5783.7921	-0.0028
10	1	10	←	9	1	9	5843.8761	0.0005
10	0	10	←	9	0	9	5918.6330	0.0013
10	2	9	←	9	2	8	5974.3889	-0.0001
10	5	6	←	9	5	5	5990.5096	0.0032
10	4	7	←	9	4	6	5991.5579	-0.0155
10	4	6	←	9	4	5	5991.6275	-0.0151
10	3	8	←	9	3	7	5993.4929	-0.0017
10	3	7	←	9	3	6	5997.0798	-0.0001
10	2	8	←	9	2	7	6040.5659	0.0005
10	1	9	←	9	1	8	6091.6302	-0.0024
5	2	3	←	4	1	3	6195.9945	0.0029

8	1	7	←	7	0	7	6377.9612	-0.0037
11	1	11	←	10	1	10	6424.7450	0.0010
5	2	4	←	4	1	4	6432.7017	0.0018
11	0	11	←	10	0	10	6497.1677	0.0044
11	2	10	←	10	2	9	6568.7646	-0.0088
11	6	6	←	10	6	5	6589.5836	-0.0026
11	5	7	←	10	5	6	6589.9052	0.0013
11	4	8	←	10	4	7	6591.4608	-0.0015
11	4	7	←	10	4	6	6591.5996	-0.0008
11	3	9	←	10	3	8	6593.6782	-0.0006
11	2	9	←	10	2	8	6654.4930	-0.0021
11	1	10	←	10	1	9	6695.3234	-0.0015
6	2	4	←	5	1	4	6746.6263	0.0027
12	1	12	←	11	1	11	7004.8031	-0.0003
12	0	12	←	11	0	11	7073.2574	0.0002
6	2	5	←	5	1	5	7094.1684	-0.0006
9	1	8	←	8	0	8	7111.0900	-0.0057
12	2	11	←	11	2	10	7162.2985	-0.0052
12	6	7	←	11	6	6	7188.7971	0.0015
12	5	8	←	11	5	7	7189.3998	0.0003
12	4	9	←	11	4	8	7191.5422	-0.0020
12	4	8	←	11	4	7	7191.7998	-0.0024
12	3	10	←	11	3	9	7193.9074	-0.0012
12	3	9	←	11	3	8	7202.8485	0.0006
12	2	10	←	11	2	9	7269.8587	-0.0006
7	2	5	←	6	1	5	7293.6431	0.0040
12	1	11	←	11	1	10	7297.2331	-0.0024
13	1	13	←	12	1	12	7584.0578	0.0011
13	0	13	←	12	0	12	7647.2993	-0.0016
13	2	12	←	12	2	11	7754.9093	-0.0045
7	2	6	←	6	1	6	7768.2531	0.0022
13	5	9	←	12	5	8	7789.0043	0.0029
13	4	9	←	12	4	8	7792.2784	-0.0048
13	3	11	←	12	3	10	7794.1514	0.0386
13	3	10	←	12	3	9	7807.3867	-0.0035
8	2	6	←	7	1	6	7839.9169	0.0025
10	1	9	←	9	0	9	7865.3605	0.0118
13	2	11	←	12	2	10	7886.1612	-0.0068
13	1	12	←	12	1	11	7897.1137	-0.0020
4	3	1	←	3	2	1	7916.1506	-0.0007
4	3	2	←	3	2	2	7918.2647	-0.0047
							RMS	**6.41 kHz**

Table S20. List of assigned transitions for phenol dimer, ^{13}C(12) isotopologue.

J'	K_a '	K_c '	←	J''	K_a''	K_c ''	ν_{obs} (MHz)	ν_{obs} - ν_{calc}
6	0	6	←	5	1	4	2251.9422	0.0130
4	1	4	←	3	1	3	2332.9881	0.0039
2	1	1	←	1	0	1	2337.8341	0.0231
4	0	4	←	3	0	3	2380.0770	-0.0034
4	2	3	←	3	2	2	2384.1935	-0.0006
4	2	2	←	3	2	1	2388.5186	-0.0016
5	1	5	←	4	1	4	2915.3914	-0.0021
5	0	5	←	4	0	4	2971.8149	-0.0003
3	1	2	←	2	0	2	2972.0450	-0.0022
5	2	4	←	4	2	3	2979.6360	0.0004
5	2	3	←	4	2	2	2988.2605	-0.0016
5	1	4	←	4	1	3	3041.7772	-0.0003
5	2	4	←	5	1	4	3134.9991	-0.0026
4	2	3	←	4	1	3	3197.1415	-0.0022
3	2	1	←	3	1	3	3401.0979	-0.0014
4	2	2	←	4	1	4	3456.6347	-0.0006
6	1	6	←	5	1	5	3497.2702	-0.0004
5	2	3	←	5	1	5	3529.5161	0.0122
6	0	6	←	5	0	5	3561.4131	-0.0004
6	2	5	←	5	2	4	3574.6733	0.0002
6	4	3	←	5	4	2	3578.6479	-0.0031
6	3	4	←	5	3	3	3579.0922	-0.0155
6	3	3	←	5	3	2	3579.3655	-0.0014
6	2	4	←	5	2	3	3589.6877	-0.0038
4	1	3	←	3	0	3	3619.5990	-0.0034
6	1	5	←	5	1	4	3648.7589	0.0001
7	1	7	←	6	1	6	4078.5347	0.0007
7	0	7	←	6	0	6	4148.5350	0.0003
7	2	6	←	6	2	5	4169.2261	-0.0009
7	5	2	←	6	5	1	4175.2437	-0.0231
7	4	4	←	6	4	3	4175.3987	0.0033
7	3	5	←	6	3	4	4176.1756	0.0008
7	3	4	←	6	3	3	4176.7574	0.0003
7	2	5	←	6	2	4	4193.0577	-0.0014
7	1	6	←	6	1	5	4254.9484	-0.0004
5	1	4	←	4	0	4	4281.2961	-0.0034
2	2	1	←	1	1	1	4527.5870	0.0001
8	1	8	←	7	1	7	4659.1130	-0.0019
8	0	8	←	7	0	7	4732.9206	-0.0003
8	2	7	←	7	2	6	4763.2193	0.0009

8	5	4	←	7	5	3	4771.9146	-0.0032
8	4	5	←	7	4	4	4772.2853	0.0078
8	3	6	←	7	3	5	4773.4325	-0.0010
8	2	6	←	7	2	5	4798.5304	-0.0020
8	1	7	←	7	1	6	4860.1795	-0.0012
6	1	5	←	5	0	5	4958.2369	-0.0062
3	2	1	←	2	1	1	5075.3150	-0.0004
3	2	2	←	2	1	2	5149.0662	-0.0016
9	1	9	←	8	1	8	5238.9583	-0.0001
9	0	9	←	8	0	8	5314.4273	-0.0011
9	2	8	←	8	2	7	5356.5701	0.0004
9	5	4	←	8	5	3	5368.6386	-0.0039
9	6	3	←	8	6	2	5368.7240	0.0033
9	4	5	←	8	4	4	5369.3602	0.0132
9	3	7	←	8	3	6	5370.9019	0.0327
9	3	6	←	8	3	5	5372.9895	-0.0022
9	2	7	←	8	2	6	5406.1627	-0.0007
9	3	7	←	9	2	7	5438.6120	-0.0019
9	1	8	←	8	1	7	5464.2711	-0.0006
8	3	6	←	8	2	6	5473.8923	-0.0158
6	3	4	←	6	2	4	5515.8810	-0.0104
6	3	3	←	6	2	5	5546.4273	0.0092
7	3	4	←	7	2	6	5553.9528	0.0045
8	3	5	←	8	2	7	5565.3291	0.0040
10	3	7	←	10	2	9	5604.5984	-0.0180
4	2	2	←	3	1	2	5637.7905	-0.0038
7	1	6	←	6	0	6	5651.7758	-0.0025
14	1	13	←	13	2	11	5680.5407	-0.0105
4	2	3	←	3	1	3	5783.1216	-0.0051
10	1	10	←	9	1	9	5818.0244	-0.0002
10	0	10	←	9	0	9	5893.0523	-0.0021
10	2	9	←	9	2	8	5949.2070	0.0019
10	6	5	←	9	6	4	5965.3568	-0.0003
10	5	6	←	9	5	5	5965.4522	0.0033
10	4	7	←	9	4	6	5966.5226	0.0002
10	4	6	←	9	4	5	5966.5918	-0.0008
10	3	8	←	9	3	7	5968.4504	-0.0022
10	3	7	←	9	3	6	5972.0736	-0.0009
10	2	8	←	9	2	7	6015.8585	-0.0033
10	1	9	←	9	1	8	6067.0211	-0.0007
5	2	3	←	4	1	3	6191.8985	0.0001
8	1	7	←	7	0	7	6363.4201	-0.0041
11	1	11	←	10	1	10	6396.2878	-0.0004
5	2	4	←	4	1	4	6429.7868	0.0087
11	0	11	←	10	0	10	6468.9455	-0.0010
11	2	10	←	10	2	9	6541.0532	0.0019

11	6	5	←	10	6	4	6562.0240	-0.0044
11	5	7	←	10	5	6	6562.3540	0.0073
11	4	8	←	10	4	7	6563.9136	-0.0013
11	4	7	←	10	4	6	6564.0536	-0.0012
11	3	9	←	10	3	8	6566.1401	0.0002
11	3	8	←	10	3	7	6571.9896	-0.0005
11	2	9	←	10	2	8	6627.3803	-0.0042
11	1	10	←	10	1	9	6668.2139	0.0014
6	2	4	←	5	1	4	6739.8156	0.0032
12	1	12	←	11	1	11	6973.7368	-0.0022
12	0	12	←	11	0	11	7042.3845	-0.0072
6	2	5	←	5	1	5	7089.0563	-0.0014
12	2	11	←	11	2	10	7132.0395	0.0017
12	6	6	←	11	6	5	7158.7343	-0.0034
12	5	8	←	11	5	7	7159.3454	0.0013
12	4	9	←	11	4	8	7161.5088	0.0061
12	4	8	←	11	4	7	7161.7626	-0.0015
12	3	10	←	11	3	9	7163.8725	-0.0005
12	3	9	←	11	3	8	7172.8989	-0.0037
12	2	10	←	11	2	9	7240.3407	-0.0048
12	1	11	←	11	1	10	7267.6078	-0.0001
7	2	5	←	6	1	5	7284.1088	-0.0040
13	1	13	←	12	1	12	7550.3768	-0.0038
13	0	13	←	12	0	12	7613.7773	-0.0044
13	2	12	←	12	2	11	7722.1035	0.0050
13	6	7	←	12	6	6	7755.4912	0.0029
13	5	9	←	12	5	8	7756.4520	0.0022
13	4	10	←	12	4	9	7759.2944	0.0015
13	4	9	←	12	4	8	7759.7571	0.0014
7	2	6	←	6	1	6	7761.0177	0.0037
13	3	11	←	12	3	10	7761.6029	0.0228
13	3	10	←	12	3	9	7774.9886	-0.0022
8	2	6	←	7	1	6	7827.6893	-0.0072
13	2	11	←	12	2	10	7854.2447	-0.0056
13	1	12	←	12	1	11	7864.9593	0.0020
4	3	1	←	3	2	1	7921.0639	0.0068
4	3	2	←	3	2	2	7923.2115	0.0202
							RMS	**6.79 kHz**

Table S21. List of assigned transitions for phenol dimer, ^{13}C(13) isotopologue.

J'	K_a '	K_c '	←	J''	K_a''	K_c ''	ν_{obs} (MHz)	ν_{obs} - ν_{calc}
6	0	6	←	5	1	4	2242.9662	-0.0045
4	1	4	←	3	1	3	2330.4029	-0.0001
2	1	1	←	1	0	1	2343.2905	-0.0233
4	0	4	←	3	0	3	2376.8495	-0.0030
4	2	3	←	3	2	2	2380.8146	-0.0055
4	2	2	←	3	2	1	2384.9847	-0.0003
4	1	3	←	3	1	2	2430.0251	-0.0023
5	1	5	←	4	1	4	2912.1941	-0.0011
5	0	5	←	4	0	4	2967.8972	-0.0015
5	2	4	←	4	2	3	2975.4368	-0.0015
3	1	2	←	2	0	2	2976.1150	-0.0008
5	3	3	←	4	3	2	2977.9444	-0.0046
5	2	3	←	4	2	2	2983.7428	-0.0016
5	1	4	←	4	1	3	3036.6462	-0.0002
6	2	5	←	6	1	5	3088.2124	0.0121
5	2	4	←	5	1	4	3161.1800	-0.0044
3	2	2	←	3	1	2	3271.6031	0.0032
6	1	6	←	5	1	5	3493.4723	-0.0003
5	2	3	←	5	1	5	3549.3212	0.0055
4	2	2	←	4	1	4	3477.7658	-0.0008
6	0	6	←	5	0	5	3556.8832	-0.0001
6	2	5	←	5	2	4	3569.6640	-0.0020
6	4	3	←	5	4	2	3573.5274	0.0049
6	3	4	←	5	3	3	3573.9458	-0.0031
6	3	3	←	5	3	2	3574.1888	-0.0040
6	2	4	←	5	2	3	3584.1288	-0.0009
4	1	3	←	3	0	3	3622.0175	0.0002
6	2	4	←	6	1	6	3639.9691	-0.0037
6	1	5	←	5	1	4	3642.6501	0.0001
7	1	7	←	6	1	6	4074.1553	-0.0002
7	0	7	←	6	0	6	4143.4735	-0.0006
7	2	6	←	6	2	5	4163.4249	-0.0014
7	5	2	←	6	5	1	4169.2906	-0.0055
7	4	4	←	6	4	3	4169.4001	0.0042
7	3	5	←	6	3	4	4170.1322	-0.0014
7	3	4	←	6	3	3	4170.6799	-0.0017
7	2	5	←	6	2	4	4186.3867	0.0011
7	1	6	←	6	1	5	4247.8908	-0.0006
5	1	4	←	4	0	4	4281.8105	-0.0008
2	2	0	←	1	1	0	4524.5469	0.0115

8	1	8	←	7	1	7	4654.1756	-0.0012
8	0	8	←	7	0	7	4727.4141	-0.0014
8	2	7	←	7	2	6	4756.6394	-0.0034
8	5	3	←	7	5	2	4765.0709	-0.0098
8	6	2	←	7	6	1	4765.3190	0.0140
8	4	5	←	7	4	4	4765.4051	0.0056
8	3	6	←	7	3	5	4766.5545	0.0515
8	3	5	←	7	3	4	4767.5952	-0.0010
8	2	6	←	7	2	5	4790.6802	0.0000
8	1	7	←	7	1	6	4852.2103	-0.0002
6	1	5	←	5	0	5	4956.5643	0.0017
3	2	1	←	2	1	1	5096.6204	0.0057
3	2	2	←	2	1	2	5169.2870	0.0025
9	1	9	←	8	1	8	5233.4801	-0.0019
9	0	9	←	8	0	8	5308.5596	0.0005
9	2	8	←	8	2	7	5349.2359	-0.0044
9	5	5	←	8	5	4	5360.9286	-0.0045
9	7	2	←	8	7	1	5361.5835	0.0111
9	3	7	←	8	3	6	5363.0426	-0.0013
9	2	7	←	8	2	6	5397.0758	0.0028
10	3	8	←	10	2	8	5435.4222	0.0186
9	1	8	←	8	1	7	5455.4331	0.0006
9	3	7	←	9	2	7	5481.1629	-0.0027
8	3	6	←	8	2	6	5515.1826	-0.0123
7	3	5	←	7	2	5	5539.3673	-0.0047
6	3	4	←	6	2	4	5555.6247	0.0007
5	3	3	←	5	2	3	5565.7980	-0.0068
5	3	2	←	5	2	4	5580.4801	-0.0037
6	3	3	←	6	2	5	5585.0117	0.0012
8	3	5	←	8	2	7	5603.2227	0.0034
7	1	6	←	6	0	6	5647.5716	0.0009
4	2	2	←	3	1	2	5658.6742	0.0034
4	2	3	←	3	1	3	5801.9226	0.0039
10	1	10	←	9	1	9	5812.0298	-0.0011
10	0	10	←	9	0	9	5886.8878	0.0000
10	2	9	←	9	2	8	5941.1412	-0.0044
10	5	6	←	9	5	5	5956.8501	-0.0114
10	7	4	←	9	7	3	5957.3028	0.0049
10	4	7	←	9	4	6	5957.8613	-0.0006
10	4	6	←	9	4	5	5957.9224	-0.0040
10	3	8	←	9	3	7	5959.7279	-0.0012
10	3	7	←	9	3	6	5963.1390	0.0008
10	2	8	←	9	2	7	6005.4928	0.0018
10	1	9	←	9	1	8	6057.3671	0.0007
5	2	3	←	4	1	3	6212.3923	0.0046
8	1	7	←	7	0	7	6356.3103	0.0032

11	1	11	←	10	1	10	6389.7988	0.0013
5	2	4	←	4	1	4	6446.9529	-0.0011
11	0	11	←	10	0	10	6462.5283	-0.0004
11	2	10	←	10	2	9	6532.2838	-0.0035
11	6	6	←	10	6	5	6552.6121	-0.0023
11	5	7	←	10	5	6	6552.8739	-0.0005
11	4	8	←	10	4	7	6554.3497	0.0009
11	4	7	←	10	4	6	6554.4794	0.0020
11	3	9	←	10	3	8	6556.5183	0.0007
11	3	8	←	10	3	7	6562.0240	-0.0013
11	2	9	←	10	2	8	6615.7201	0.0051
11	1	10	←	10	1	9	6657.8031	0.0000
6	2	4	←	5	1	4	6759.8646	-0.0063
12	1	12	←	11	1	11	6966.7713	0.0012
12	0	12	←	11	0	11	7035.7471	0.0037
6	2	5	←	5	1	5	7104.4227	-0.0021
12	2	11	←	11	2	10	7122.5935	-0.0037
12	6	6	←	11	6	5	7148.4382	-0.0081
12	7	5	←	11	7	4	7148.7302	-0.0125
12	5	8	←	11	5	7	7148.9798	0.0004
12	4	9	←	11	4	8	7151.0201	-0.0010
12	4	8	←	11	4	7	7151.2623	0.0009
12	3	10	←	11	3	9	7153.3537	-0.0009
12	3	9	←	11	3	8	7161.8617	0.0034
12	2	10	←	11	2	9	7227.3956	0.0079
12	1	11	←	11	1	10	7256.5200	0.0024
7	2	5	←	6	1	5	7303.6086	0.0021
3	3	0	←	2	2	0	7362.0400	0.0157
3	3	1	←	2	2	1	7362.4186	-0.0188
13	1	13	←	12	1	12	7542.9508	0.0008
13	0	13	←	12	0	12	7606.9005	0.0021
13	2	12	←	12	2	11	7712.0057	-0.0049
13	6	8	←	12	6	7	7744.3089	-0.0048
13	5	8	←	12	5	7	7745.1874	-0.0043
13	4	10	←	12	4	9	7747.8875	0.0020
13	4	9	←	12	4	8	7748.3134	0.0023
13	3	11	←	12	3	10	7750.1741	0.0016
13	4	10	←	13	3	10	7758.5113	0.0068
13	3	10	←	12	3	9	7762.8130	0.0057
7	2	6	←	6	1	6	7774.3795	0.0010
8	2	6	←	7	1	6	7846.3889	-0.0064
4	3	1	←	3	2	1	7956.6058	-0.0099
4	3	2	←	3	2	2	7958.6651	-0.0058
							RMS	**7.11 kHz**

Table S22. List of assigned transitions for phenol dimer, ^{13}C(14) isotopologue.

J'	K_a '	K_c '	←	J''	K_a''	K_c ''	ν_{obs} (MHz)	ν_{obs} - ν_{calc}
6	0	6	←	5	1	4	2256.8090	0.0029
4	1	4	←	3	1	3	2338.2504	-0.0032
4	0	4	←	3	0	3	2384.7867	0.0010
4	2	3	←	3	2	2	2388.7759	0.0002
4	2	2	←	3	2	1	2392.9676	0.0001
4	1	3	←	3	1	2	2438.0854	0.0007
5	1	5	←	4	1	4	2922.0048	0.0010
5	0	5	←	4	0	4	2977.7959	0.0002
3	1	2	←	2	0	2	2979.7939	-0.0009
5	2	4	←	4	2	3	2985.3793	-0.0001
5	3	3	←	4	3	2	2987.8994	-0.0028
5	3	2	←	4	3	1	2988.0030	0.0082
5	2	3	←	4	2	2	2993.7376	-0.0012
7	2	6	←	7	1	6	2995.7106	0.0099
5	1	4	←	4	1	3	3046.7114	-0.0014
6	2	5	←	6	1	5	3080.3259	-0.0074
10	1	9	←	9	2	7	3149.1579	-0.0002
5	2	4	←	5	1	4	3153.4654	0.0008
4	2	3	←	4	1	3	3214.8019	0.0039
8	0	8	←	7	1	6	3240.5135	0.0065
3	2	2	←	3	1	2	3264.1130	0.0060
3	2	1	←	3	1	3	3416.0129	-0.0021
4	2	2	←	4	1	4	3470.7236	-0.0052
6	1	6	←	5	1	5	3505.2364	0.0002
5	2	3	←	5	1	5	3542.4585	-0.0053
6	0	6	←	5	0	5	3568.7331	0.0012
6	2	5	←	5	2	4	3581.5900	-0.0005
6	4	3	←	5	4	2	3585.4662	0.0059
6	3	4	←	5	3	3	3585.8966	0.0009
6	3	3	←	5	3	2	3586.1409	-0.0015
6	2	4	←	5	2	3	3596.1453	-0.0010
4	1	3	←	3	0	3	3627.7969	0.0025
6	2	4	←	6	1	6	3633.3643	-0.0095
6	1	5	←	5	1	4	3654.7209	-0.0010
9	0	9	←	8	1	7	3698.3887	-0.0209
7	1	7	←	6	1	6	4087.8727	0.0015
7	0	7	←	6	0	6	4157.2605	-0.0001
7	2	6	←	6	2	5	4177.3300	-0.0013
7	5	2	←	6	5	1	4183.2117	-0.0039
7	4	4	←	6	4	3	4183.3267	0.0005

7	3	5	←	6	3	4	4184.0760	0.0006
7	3	4	←	6	3	3	4184.6279	-0.0015
7	2	5	←	6	2	4	4200.4342	-0.0014
7	1	6	←	6	1	5	4261.9623	-0.0015
5	1	4	←	4	0	4	4289.7333	0.0118
2	2	0	←	1	1	0	4521.1472	-0.0060
2	2	1	←	1	1	1	4545.7022	-0.0022
8	1	8	←	7	1	7	4669.8408	0.0000
8	0	8	←	7	0	7	4743.1250	-0.0010
8	2	7	←	7	2	6	4772.5245	-0.0008
8	5	4	←	7	5	3	4780.9935	0.0027
8	4	5	←	7	4	4	4781.3294	0.0059
8	3	6	←	7	3	5	4782.4387	-0.0021
8	3	5	←	7	3	4	4783.5448	-0.0012
8	2	6	←	7	2	5	4806.7731	-0.0015
8	1	7	←	7	1	6	4868.2760	-0.0018
6	1	5	←	5	0	5	4966.6685	0.0208
3	2	1	←	2	1	1	5095.1798	-0.0005
3	2	2	←	2	1	2	5167.9849	-0.0068
9	1	9	←	8	1	8	5251.0904	-0.0005
9	0	9	←	8	0	8	5326.1794	-0.0011
9	2	8	←	8	2	7	5367.0954	-0.0013
9	5	5	←	8	5	4	5378.8343	-0.0008
9	6	3	←	8	6	2	5378.9330	-0.0002
9	4	5	←	8	4	4	5379.5041	0.0049
9	3	7	←	8	3	6	5380.9761	-0.0025
9	3	6	←	8	3	5	5382.9971	-0.0009
9	2	7	←	8	2	6	5415.2198	-0.0017
9	1	8	←	8	1	7	5473.4858	-0.0017
9	3	7	←	9	2	7	5468.3133	0.0010
8	3	6	←	8	2	6	5502.5607	0.0054
7	3	5	←	7	2	5	5526.8973	0.0083
6	3	4	←	6	2	4	5543.2484	-0.0009
5	3	3	←	5	2	3	5553.4951	-0.0047
4	3	2	←	4	2	2	5559.3211	-0.0153
5	3	2	←	5	2	4	5568.2741	0.0005
6	3	3	←	6	2	5	5572.8207	-0.0048
8	3	5	←	8	2	7	5591.1475	0.0034
9	3	6	←	9	2	8	5607.0485	0.0031
4	2	2	←	3	1	2	5659.1728	-0.0008
7	1	6	←	6	0	6	5659.8638	-0.0158
4	2	3	←	3	1	3	5802.7163	0.0249
10	1	10	←	9	1	9	5831.5806	-0.0007
10	0	10	←	9	0	9	5906.4098	0.0001
10	2	9	←	9	2	8	5960.9708	-0.0011
10	6	5	←	9	6	4	5976.6864	-0.0058

10	5	6	←	9	5	5	5976.7594	0.0029
10	3	8	←	9	3	7	5979.6618	0.0007
10	3	7	←	9	3	6	5983.1076	0.0000
10	2	8	←	9	2	7	6025.6985	-0.0016
5	2	3	←	4	1	3	6214.8252	-0.0026
8	1	7	←	7	0	7	6370.9134	0.0166
11	1	11	←	10	1	10	6411.2868	0.0007
5	2	4	←	4	1	4	6449.8152	-0.0021
11	0	11	←	10	0	10	6483.9426	-0.0017
11	2	10	←	10	2	9	6554.0791	-0.0002
11	6	5	←	10	6	4	6574.4845	0.0025
11	5	7	←	10	5	6	6574.7641	0.0006
11	4	8	←	10	4	7	6576.2632	0.0002
11	4	7	←	10	4	6	6576.3956	0.0019
11	3	9	←	10	3	8	6578.4478	0.0007
11	3	8	←	10	3	7	6584.0147	-0.0002
11	2	9	←	10	2	8	6637.9868	-0.0002
11	1	10	←	10	1	9	6679.8044	-0.0008
6	2	4	←	5	1	4	6764.2603	-0.0009
12	1	12	←	11	1	11	6990.1949	0.0012
12	0	12	←	11	0	11	7059.0504	0.0000
9	1	8	←	8	0	8	7101.2501	-0.0082
6	2	5	←	5	1	5	7109.3948	-0.0092
12	2	11	←	11	2	10	7146.3505	0.0004
12	7	5	←	11	7	4	7172.5696	-0.0091
12	4	9	←	11	4	8	7174.9365	0.0011
12	4	8	←	11	4	7	7175.1779	-0.0016
12	3	10	←	11	3	9	7177.2797	-0.0012
12	3	9	←	11	3	8	7185.8778	0.0008
12	2	10	←	11	2	9	7251.7204	0.0004
12	1	11	←	11	1	10	7280.4767	0.0011
7	2	5	←	6	1	5	7309.9766	0.0017
3	3	0	←	2	2	0	7355.7554	-0.0059
13	1	13	←	12	1	12	7568.3071	0.0009
13	0	13	←	12	0	12	7632.1002	0.0014
13	2	12	←	12	2	11	7737.7183	-0.0011
13	5	9	←	12	5	8	7771.0673	0.0012
13	4	10	←	12	4	9	7773.8045	0.0028
13	4	9	←	12	4	8	7774.2362	0.0021
7	2	6	←	6	1	6	7781.4947	-0.0044
13	3	10	←	12	3	9	7788.8700	0.0045
10	1	9	←	9	0	9	7852.4722	-0.0056
8	2	6	←	7	1	6	7854.7871	0.0014
13	2	11	←	12	2	10	7866.4285	0.0004
13	1	12	←	12	1	11	7879.1727	0.0030

4	3	1	←	3	2	1	7952.3388	0.0041
4	3	2	←	3	2	2	7954.4119	0.0090
							RMS	**5.38 kHz**

Table S23. List of assigned transitions for phenol dimer, ^{18}O(7) isotopologue.

J'	K_a '	K_c '	←	J''	K_a''	K_c ''	ν_{obs} (MHz)	ν_{obs} - ν_{calc}
4	1	4	←	3	1	3	2342.0405	-0.0116
4	0	4	←	3	0	3	2390.6414	-0.0056
4	1	3	←	3	1	2	2446.8417	-0.0193
5	1	5	←	4	1	4	2926.6556	-0.0026
5	0	5	←	4	0	4	2984.7353	0.0056
5	2	3	←	4	2	2	3002.6825	0.0087
5	1	4	←	4	1	3	3057.5905	0.0129
6	1	6	←	5	1	5	3510.6807	-0.0083
6	0	6	←	5	0	5	3576.4985	0.0075
6	2	5	←	5	2	4	3590.9456	0.0009
6	5	1	←	5	5	0	3595.2385	0.0046
6	3	4	←	5	3	3	3595.7532	-0.0070
6	2	4	←	5	2	3	3607.3340	0.0004
6	1	5	←	5	1	4	3667.6186	0.0191
7	1	7	←	6	1	6	4094.0537	-0.0042
7	0	7	←	6	0	6	4165.5762	0.0058
7	2	6	←	6	2	5	4188.1120	0.0007
7	3	5	←	6	3	4	4195.6485	-0.0109
7	3	4	←	6	3	3	4196.3194	-0.0105
7	2	5	←	6	2	4	4214.0936	-0.0032
7	1	6	←	6	1	5	4276.7801	0.0220
8	1	8	←	7	1	7	4676.6834	-0.0097
8	0	8	←	7	0	7	4751.7129	0.0066
8	2	7	←	7	2	6	4784.6625	-0.0076
8	2	6	←	7	2	5	4823.1292	0.0011
8	1	7	←	7	1	6	4884.8920	0.0223
9	1	9	←	8	1	8	5258.5298	-0.0086
9	0	9	←	8	0	8	5334.7788	0.0077
9	2	8	←	8	2	7	5380.5429	0.0057
9	5	5	←	8	5	4	5393.5928	0.0010
9	3	7	←	8	3	6	5396.0538	-0.0121
9	3	6	←	8	3	5	5398.4913	-0.0173
9	2	7	←	8	2	6	5434.4578	0.0018
9	1	8	←	8	1	7	5491.7464	0.0149
10	1	10	←	9	1	9	5839.5453	-0.0086
10	0	10	←	9	0	9	5914.8055	0.0064
10	2	9	←	9	2	8	5975.6292	-0.0020
10	3	8	←	9	3	7	5996.5068	-0.0135
10	3	7	←	9	3	6	6000.6679	-0.0193
10	2	8	←	9	2	7	6047.9386	-0.0069

10	1	9	←	9	1	8	6097.1368	0.0158
11	1	11	←	10	1	10	6419.7109	-0.0060
11	0	11	←	10	0	10	6491.9993	0.0064
11	2	10	←	10	2	9	6569.8612	-0.0123
11	4	8	←	10	4	7	6594.7358	-0.0088
11	2	9	←	10	2	8	6663.2867	-0.0039
11	1	10	←	10	1	9	6700.8136	0.0183
12	1	12	←	11	1	11	6999.0179	-0.0033
12	0	12	←	11	0	11	7066.7147	0.0117
12	2	11	←	11	2	10	7163.1823	-0.0065
12	10	2	←	11	10	1	7195.5414	0.0078
12	2	10	←	11	2	9	7280.0238	-0.0093
12	1	11	←	11	1	10	7302.5053	0.0132
13	1	13	←	12	1	12	7577.4793	0.0039
13	0	13	←	12	0	12	7639.3953	0.0135
13	2	12	←	12	2	11	7755.4911	-0.0156
13	2	11	←	12	2	10	7897.5965	-0.0107
13	1	12	←	12	1	11	7901.9447	0.0107
8	0	8	←	7	1	6	3251.5263	0.0061
4	2	2	←	3	1	2	5587.9434	-0.0007
							RMS	**10.4 kHz**

Table S24. List of assigned transitions for phenol dimer, ^{18}O(8) isotopologue.

J'	K_a '	K_c '	←	J''	K_a''	K_c ''	ν_{obs} (MHz)	ν_{obs} - ν_{calc}
4	0	4	←	3	0	3	2391.9009	-0.0021
4	2	2	←	3	2	1	2401.0993	-0.0090
4	1	3	←	3	1	2	2448.1441	-0.0008
5	1	5	←	4	1	4	2928.2043	0.0120
5	0	5	←	4	0	4	2986.3026	0.0023
5	2	3	←	4	2	2	3004.2416	0.0003
5	1	4	←	4	1	3	3059.1815	-0.0006
6	1	6	←	5	1	5	3512.5338	0.0029
6	0	6	←	5	0	5	3578.3791	0.0024
6	2	5	←	5	2	4	3592.8271	0.0008
6	3	4	←	5	3	3	3597.6408	-0.0003
6	3	3	←	5	3	2	3597.9357	-0.0037
6	2	4	←	5	2	3	3609.2154	0.0015
6	1	5	←	5	1	4	3669.5286	0.0046
7	1	7	←	6	1	6	4096.2084	0.0000
7	0	7	←	6	0	6	4167.7720	0.0002
7	2	6	←	6	2	5	4190.3079	0.0016
7	4	4	←	6	4	3	4196.9823	-0.0010
7	3	5	←	6	3	4	4197.8541	0.0005
7	3	4	←	6	3	3	4198.5190	-0.0044
7	2	5	←	6	2	4	4216.2970	0.0074
7	1	6	←	6	1	5	4279.0023	-0.0005
8	1	8	←	7	1	7	4679.1524	-0.0002
8	0	8	←	7	0	7	4754.2251	0.0014
8	2	7	←	7	2	6	4787.1844	0.0061
8	3	5	←	7	3	4	4799.6091	-0.0015
8	2	6	←	7	2	5	4825.6284	-0.0047
8	1	7	←	7	1	6	4887.4333	-0.0009
9	1	9	←	8	1	8	5261.3130	0.0053
9	0	9	←	8	0	8	5337.6035	-0.0016
9	2	8	←	8	2	7	5383.3541	-0.0046
9	4	6	←	8	4	5	5397.2005	0.0012
9	3	7	←	8	3	6	5398.8830	-0.0030
9	2	7	←	8	2	6	5437.2746	0.0016
9	1	8	←	8	1	7	5494.6251	0.0094
10	1	10	←	9	1	9	5842.6344	0.0004
10	0	10	←	9	0	9	5917.9460	-0.0039
10	2	9	←	9	2	8	5978.7345	-0.0315
10	5	6	←	9	5	5	5996.3409	-0.0145
10	3	8	←	9	3	7	5999.6527	-0.0008

10	1	9	←	9	1	8	6100.3288	0.0036
11	1	11	←	10	1	10	6423.1122	0.0031
11	0	11	←	10	0	10	6495.4613	0.0009
11	2	10	←	10	2	9	6573.3275	0.0059
11	5	7	←	10	5	6	6596.3982	-0.0125
11	8	3	←	10	8	2	6597.0527	0.0212
11	3	9	←	10	3	8	6600.5220	-0.0039
11	3	8	←	10	3	7	6607.2429	-0.0027
11	2	9	←	10	2	8	6666.7403	0.0071
11	1	10	←	10	1	9	6704.3226	0.0028
12	1	12	←	11	1	11	7002.7295	0.0031
12	0	12	←	11	0	11	7070.4850	-0.0016
12	2	11	←	11	2	10	7166.9592	0.0087
12	5	8	←	11	5	7	7196.5650	-0.0197
12	4	9	←	11	4	8	7199.0040	-0.0028
12	3	10	←	11	3	9	7201.4416	0.0053
12	3	9	←	11	3	8	7211.8047	0.0045
12	2	10	←	11	2	9	7283.7921	0.0021
12	1	11	←	11	1	10	7306.3408	0.0033
13	1	13	←	12	1	12	7581.4979	0.0030
13	0	13	←	12	0	12	7643.4780	-0.0030
13	2	12	←	12	2	11	7759.5916	0.0093
13	4	9	←	12	4	8	7800.6024	-0.0116
13	3	10	←	12	3	9	7817.6855	0.0055
13	2	11	←	12	2	10	7901.6789	-0.0013
13	1	12	←	12	1	11	7906.1008	-0.0008
7	1	6	←	6	0	6	5669.4732	0.0048
8	1	7	←	7	0	7	6389.1277	-0.0031
3	1	2	←	2	0	2	2965.8015	-0.0016
							RMS	**7.02 kHz**

Table S25. Carbon coordinates for the phenol trimer for the r_s and $r_m^{(1)}$ geometries, compared to the M06-2X/6-311++g(d,p) theoretical geometry.

	M06-2X/6-311++g(d,p)			rs structure			$r_m^{(1)}$ structure		
	a	**b**	**c**	**a**	**b**	**c**	**a**	**b**	**c**
C-OH									
C1	-1.73(29)	1.63(40)	-0.7787(20)	-1.7372(69)	1.4863(50)	-0.7690(97)	-1.73(29)	1.63(40)	-0.7787(20)
C1'	2.19(24)	0.84(48)	-0.7787(20)	2.1571(66)	0.7587(87)	-0.7690(97)	2.19(24)	0.84(48)	-0.7787(20)
C1''	-0.45(25)	-2.168(29)	-0.7787(20)	-0.4170(76)	-2.2458(49)	-0.7690(97)	-0.45(25)	-2.168(29)	-0.7787(20)
6-ortho									
C2	-3.12(28)	1.53(38)	-0.6640(19)	-3.123(71)	1.3689(46)	-0.662(10)	-3.12(28)	1.53(38)	-0.6640(19)
C2'	2.80(25)	2.08(44)	-0.6640(19)	2.7471(64)	2.0192(68)	-0.662(10)	2.80(25)	2.08(44)	-0.6640(19)
C2''	0.32(29)	-3.32(42)	-0.6640(19)	0.3782(66)	-3.3868(47)	-0.662(10)	0.32(29)	-3.32(42)	-0.6640(19)
2-ortho									
C3	-1.01(32)	2.04(22)	0.2993(19)	-0.9942(50)	1.9760(42)	0.304(11)	-1.01(32)	2.04(22)	0.2993(19)
C3'	2.17(25)	-0.10(56)	0.2993(19)	2.208(50)	-0.1281(41)	0.304(11)	2.17(25)	-0.10(56)	0.2993(19)
C3''	-1.27(39)	-1.77(32)	0.2993(19)	-1.2492(34)	-1.8378(35)	0.304(11)	-1.27(39)	-1.77(32)	0.2993(19)
5-meta									
C4	-3.78(43)	1.83(41)	0.5293(25)	-3.749(11)	1.709(11)	0.533(11)	-3.78(43)	1.83(41)	0.5293(25)
C4'	3.36(52)	2.39(55)	0.5293(25)	3.359(10)	2.389(13)	0.533(11)	3.36(52)	2.39(55)	0.5293(25)
C4''	0.28(22)	-4.08(37)	0.5293(25)	0.396(10)	-4.104(11)	0.533(11)	0.28(22)	-4.08(37)	0.5293(25)
3-meta									
C5	-1.69(72)	2.34(23)	1.4884(52)	-1.658(12)	2.3821(56)	1.462(20)	-1.69(72)	2.34(23)	1.4884(52)
C5'	2.74(62)	0.231(72)	1.4884(52)	2.890(12)	0.2430(58)	1.462(20)	2.74(62)	0.231(72)	1.4884(52)
C5''	-1.30(31)	-2.54(48)	1.4884(52)	-1.233(19)	-2.624(52)	1.462(20)	-1.30(31)	-2.54(48)	1.4884(52)
para									
C6	-3.07(33)	2.24(43)	1.6121(12)	-3.046(18)	2.301(12)	1.552(24)	-3.07(33)	2.24(43)	1.6121(12)
C6'	3.34(42)	1.47(63)	1.6121(12)	3.515(18)	1.485(47)	1.552(24)	3.34(42)	1.47(63)	1.6121(12)
C6''	-0.52(23)	-3.70(52)	1.6121(12)	-0.481(18)	-3.794(12)	1.552(24)	-0.52(23)	-3.70(52)	1.6121(12)

Table S26. Full coordinates for the $r_m^{(1)}$ geometry of phenol trimer. [4]

O	1.60518197	0.60583237	-1.87184885
H	1.24856482	-0.29944156	-1.93045199
O	-1.12613254	1.26203234	-1.9508909
H	-0.16226235	1.40481736	-1.91717611
O	-0.32470642	-1.43077258	-2.02677812
H	-0.93092263	-0.66721536	-2.0288487
C	-0.44937977	-2.16864333	-0.8800169
C	0.32386282	-3.3259125	-0.78797361
C	-1.26593399	-1.77312718	0.17988837
C	0.28490764	-4.08462241	0.3782844
H	0.94404384	-3.61118029	-1.63172879
C	-1.29524	-2.54366211	1.34104127
H	-1.86110492	-0.86572241	0.10682563
C	-0.5204044	-3.69708569	1.44932259
H	0.88956804	-4.98378312	0.44803271
H	-1.92732995	-2.23040102	2.16541727
H	-0.54787887	-4.29113384	2.35714359
C	-1.73028824	1.63068591	-0.77872136
C	-1.00605313	2.03940768	0.34096566
C	-3.12055412	1.53123349	-0.72796724
C	-1.68668641	2.34110668	1.51955891
H	0.07832442	2.10801404	0.29925829
C	-3.78619103	1.8336969	0.45624068
H	-3.65763264	1.21616821	-1.61741119
C	-3.07441433	2.23701356	1.58625112
H	-1.11932721	2.65396832	2.39004965
H	-4.86900426	1.75363652	0.49354822
H	-3.59712258	2.47146494	2.50785713
C	2.19818565	0.83509928	-0.65916039
C	2.16588475	-0.09707603	0.37829362
C	2.80365798	2.07945189	-0.47839855
C	2.73905502	0.2317278	1.60618201
H	1.68658567	-1.06287874	0.23545622
C	3.36957518	2.3932793	0.75362502
H	2.81816373	2.78082472	-1.30634949
C	3.33900538	1.47408458	1.80267676
H	2.7080428	-0.49440323	2.41248652
H	3.83828129	3.36276677	0.89219494
H	3.78015119	1.72226752	2.76189655

[4] Coordinate values in this geometry deviate slightly from the $r_m^{(1)}$ coordinates stated in S24. This is because phenol trimer is a symmetric top, so the moment of inertia tensor is invariant upon rotation around the c axis (the symmetry axis). The values in S24 are rotated to match geometries as closely as possible.

Table S27. Full coordinates for the M06-2X/6-311++g(d,p) geometry of phenol trimer.

O	1.57396291	0.47962632	-1.95904512
H	1.21393329	-0.4266572	-1.98048427
O	-1.15817342	1.13927893	-1.98142103
H	-0.19305477	1.28059141	-1.97832017
O	-0.36312678	-1.55660072	-1.99997044
H	-0.96794338	-0.79137167	-2.0072764
C	-0.45715077	-2.25965451	-0.82850188
C	0.31654597	-3.4157037	-0.72357267
C	-1.24263215	-1.83076902	0.24141372
C	0.30974898	-4.13953519	0.46521586
H	0.91278397	-3.72702695	-1.57539355
C	-1.24073602	-2.56744858	1.42513333
H	-1.83840152	-0.92494177	0.15820169
C	-0.46563307	-3.71906131	1.54656261
H	0.91422324	-5.03782284	0.54449925
H	-1.84893551	-2.22818178	2.25788598
H	-0.46807593	-4.28553628	2.47163203
C	-1.7285677	1.54376203	-0.80392013
C	-0.97225097	1.98354657	0.28245746
C	-3.11729133	1.44922789	-0.71130213
C	-1.61980109	2.321496	1.47004432
H	0.11066646	2.04858423	0.2086351
C	-3.74940446	1.78815727	0.48149081
H	-3.67877728	1.10924417	-1.57568913
C	-3.0055036	2.22312692	1.57909675
H	-1.02799653	2.65832951	2.31550033
H	-4.83011375	1.71191088	0.55112797
H	-3.50159907	2.48601376	2.50723105
C	2.20085881	0.74279037	-0.77025971
C	2.1958575	-0.15811959	0.29462457
C	2.81244017	1.99012368	-0.64299546
C	2.80362149	0.20485566	1.49577626
H	1.71144492	-1.12640361	0.19383639
C	3.41330022	2.33911763	0.56297561
H	2.8048891	2.66709724	-1.49132889
C	3.41025297	1.45109303	1.63941779
H	2.79342691	-0.49633421	2.32445806
H	3.88693143	3.31119554	0.65959097
H	3.87918142	1.72674012	2.57791522

Table S28. Assigned transitions for phenol trimer, parent species.

J'	K'	←	J''	K''	ν_{obs} (MHz)	$\nu_{obs} - \nu_{calc}$
4	0	←	3	0	2258.2205	0.0005
5	0	←	4	0	2822.7561	-0.0003
6	0	←	5	0	3387.2801	-0.0004
7	0	←	6	0	3951.7896	-0.0002
8	0	←	7	0	4516.2810	-0.0007
9	0	←	8	0	5080.7525	-0.0014
10	0	←	9	0	5645.2035	-0.0004
11	0	←	10	0	6209.6303	0.0012
12	0	←	11	0	6774.0283	0.0011
12	11	←	11	11	6774.4230	0.0009
13	0	←	12	0	7338.3971	0.0016
13	10	←	12	10	7338.7464	-0.0028
13	11	←	12	11	7338.8250	0.0015
13	12	←	12	12	7338.9069	0.0022
14	0	←	13	0	7902.7321	0.0003
14	10	←	13	10	7903.1104	-0.0022
14	11	←	13	11	7903.1943	0.0016
14	12	←	13	12	7903.2802	0.0000
14	13	←	13	13	7903.3751	-0.0004

Table S29. Assigned transitions for phenol trimer, 1-^{13}C isotopologue.

J'	K_a '	K_c '	←	J''	K_a''	K_c ''	ν_{obs} (MHz)	$\nu_{obs} - \nu_{calc}$
4	3	1	←	3	2	1	2252.2513	0.0082
4	4	0	←	3	3	0	2254.0744	0.0080
4	4	1	←	3	3	1	2255.7793	-0.0125
5	4	1	←	4	3	1	2815.3013	0.0033
5	3	2	←	4	2	2	2817.3789	-0.0020
5	5	0	←	4	4	0	2817.6060	-0.0055
5	5	1	←	4	4	1	2819.7250	-0.0076
6	5	1	←	5	4	1	3378.3541	0.0048
6	4	2	←	5	3	2	3380.7734	0.0000
6	3	3	←	5	2	3	3380.9412	0.0046
6	5	2	←	5	4	2	3380.9977	0.0059
6	6	0	←	5	5	0	3381.1791	0.0035
6	6	1	←	5	5	1	3383.6625	-0.0060
7	6	1	←	6	5	1	3941.4021	0.0060
7	5	2	←	6	4	2	3944.1143	-0.0063
7	4	3	←	6	3	3	3944.3874	0.0109
7	6	2	←	6	5	2	3944.4759	0.0065
7	7	0	←	6	6	0	3944.7658	0.0037
7	7	1	←	6	6	1	3947.5923	-0.0060
8	7	1	←	7	6	1	4504.4433	0.0054

8	6	2	←	7	5	2	4507.4175	0.0021
8	7	2	←	7	6	2	4507.9331	-0.0041
8	8	0	←	7	7	0	4508.3785	0.0043
8	8	1	←	7	7	1	4511.5166	-0.0042
9	8	1	←	8	7	1	5067.4764	0.0020
9	7	2	←	8	6	2	5070.6518	0.0008
9	6	3	←	8	5	3	5071.1906	0.0075
9	8	2	←	8	7	2	5071.3974	0.0035
9	9	0	←	8	8	0	5072.0136	-0.0013
9	9	1	←	8	8	1	5075.4298	-0.0049
10	9	1	←	9	8	1	5630.5091	0.0038
10	8	2	←	9	7	2	5633.8243	0.0029
10	7	3	←	9	6	3	5634.5518	0.0094
10	10	0	←	9	9	0	5635.6864	-0.0001
10	10	1	←	9	9	1	5639.3338	-0.0048
11	10	1	←	10	9	1	6193.5275	-0.0028
11	9	2	←	10	8	2	6196.9208	-0.0001
11	10	2	←	10	9	2	6198.2640	-0.0041
11	11	0	←	10	10	0	6199.3851	-0.0055
11	11	1	←	10	10	1	6203.2293	-0.0016
12	11	1	←	11	10	1	6756.5403	-0.0090
12	2	10	←	11	1	10	6761.6796	-0.0006
12	2	11	←	11	1	11	6761.7602	0.0095
12	12	0	←	11	11	0	6763.1290	0.0010
12	12	1	←	11	11	1	6767.1128	0.0030
13	12	1	←	12	11	1	7319.5525	-0.0098
13	11	2	←	12	10	2	7322.8802	-0.0105
13	10	3	←	12	9	3	7324.3923	-0.0065
13	11	3	←	12	10	3	7324.4792	-0.0014
13	9	4	←	12	8	4	7324.5947	-0.0024
13	8	5	←	12	7	5	7324.6831	-0.0029
13	6	7	←	12	5	7	7324.8303	0.0134
13	4	9	←	12	3	9	7324.9461	-0.0010
13	1	12	←	12	0	12	7325.1846	0.0060
13	13	0	←	12	12	0	7326.8995	0.0011
13	13	1	←	12	12	1	7330.9715	-0.0021
14	13	1	←	13	12	1	7882.5601	-0.0095
14	9	5	←	13	8	5	7887.9483	-0.0058
14	5	9	←	13	4	9	7888.2467	0.0000
14	4	10	←	13	3	10	7888.3244	-0.0003
14	3	11	←	13	2	11	7888.4205	0.0123
14	1	13	←	13	0	13	7888.5877	-0.0070
14	14	1	←	13	13	1	7894.8286	0.0082
							RMS	**5.96 kHz**

Table S30. Assigned transitions for phenol trimer, 2-^{13}C isotopologue.

J'	K_a '	K_c '	←	J''	K_a''	K_c ''	ν_{obs} (MHz)	$\nu_{obs} - \nu_{calc}$
4	3	1	←	3	2	1	2253.2179	0.0066
4	4	1	←	3	3	1	2256.4882	-0.0006
5	4	1	←	4	3	1	2816.5079	0.0013
5	3	2	←	4	2	2	2818.4466	0.0062
5	5	0	←	4	4	0	2818.6369	0.0007
5	5	1	←	4	4	1	2820.6027	0.0005
6	5	1	←	5	4	1	3379.8030	0.0063
6	4	2	←	5	3	2	3382.0544	0.0012
6	6	1	←	5	5	1	3384.7049	-0.0046
7	6	1	←	6	5	1	3943.0852	0.0041
7	5	2	←	6	4	2	3945.6254	0.0003
7	4	3	←	6	3	3	3945.8527	0.0079
7	7	0	←	6	6	0	3946.1707	-0.0003
7	7	1	←	6	6	1	3948.8040	-0.0056
8	7	1	←	7	6	1	4506.3627	0.0039
8	6	2	←	7	5	2	4509.1483	-0.0015
8	5	3	←	7	4	3	4509.4915	0.0177
8	8	0	←	7	7	0	4509.9633	-0.0030
8	8	1	←	7	7	1	4512.9018	0.0009
9	8	1	←	8	7	1	5069.6323	0.0033
9	7	2	←	8	6	2	5072.6185	-0.0025
9	6	4	←	8	5	4	5073.1378	0.0009
9	9	0	←	8	8	0	5073.7768	-0.0065
9	9	1	←	8	8	1	5076.9802	-0.0017
10	8	2	←	9	7	2	5636.0308	-0.0022
10	7	3	←	9	6	3	5636.6537	0.0020
10	10	0	←	9	9	0	5637.6216	-0.0021
10	10	1	←	9	9	1	5641.0516	0.0004
11	10	1	←	10	9	1	6196.1685	0.0238
11	9	2	←	10	8	2	6199.3851	0.0046
11	11	0	←	10	10	0	6201.4840	-0.0050
11	11	1	←	10	10	1	6205.1036	-0.0034
12	11	1	←	11	10	1	6759.3913	0.0024
12	10	2	←	11	9	2	6762.6565	-0.0024
12	9	3	←	11	8	3	6763.7173	0.0186
12	12	0	←	11	11	0	6765.3749	-0.0046
12	2	11	←	11	1	11	6764.2603	0.0021
12	12	1	←	11	11	1	6769.1458	-0.0018
13	12	1	←	12	11	1	7322.6088	-0.0149
13	11	2	←	12	10	2	7325.8553	-0.0094
13	8	5	←	12	7	5	7327.4091	-0.0049
13	5	9	←	12	4	9	7327.6591	-0.0061
13	6	8	←	12	5	8	7327.5944	-0.0052

13	2	11	←	12	1	11	7327.8197	0.0073
13	1	12	←	12	0	12	7327.9251	0.0301
13	13	0	←	12	12	0	7329.2886	-0.0064
13	13	1	←	12	12	1	7333.1762	0.0051
14	12	2	←	13	11	2	7888.9779	-0.0169
14	13	1	←	13	12	1	7885.8265	-0.0221
14	12	3	←	13	11	3	7890.6945	0.0161
14	10	4	←	13	9	4	7890.7840	-0.0154
14	2	12	←	13	1	12	7891.4211	-0.0028
14	14	0	←	13	13	0	7893.2373	0.0030
							RMS	**9.10 kHz**

Table S31. Assigned transitions for phenol trimer, 3-^{13}C isotopologue.

J'	K_a '	K_c '	←	J''	K_a''	K_c ''	ν_{obs} (MHz)	ν_{obs} - ν_{calc}
4	3	1	←	3	2	1	2247.3098	0.0054
4	4	0	←	3	3	0	2250.2342	0.0078
4	4	1	←	3	3	1	2252.8989	-0.0018
5	4	1	←	4	3	1	2809.1889	0.0461
5	3	2	←	4	2	2	2812.3051	0.0075
5	4	2	←	4	3	2	2812.6006	-0.0091
5	5	0	←	4	4	0	2812.8883	0.0066
5	5	1	←	4	4	1	2816.1288	-0.0070
6	5	1	←	5	4	1	3370.9891	-0.0008
6	4	2	←	5	3	2	3374.5894	0.0007
6	5	2	←	5	4	2	3375.1448	0.0113
6	6	0	←	5	5	0	3375.5992	-0.0025
6	6	1	←	5	5	1	3379.3759	-0.0010
7	6	1	←	6	5	1	3932.8478	-0.0005
7	5	2	←	6	4	2	3936.7958	0.0060
7	4	3	←	6	3	3	3937.4128	0.0033
7	7	1	←	6	6	1	3942.6250	0.0004
8	6	2	←	7	5	2	4498.8879	-0.0006
8	7	2	←	7	6	2	4500.1909	0.0065
8	8	0	←	7	7	0	4501.2784	-0.0028
8	8	1	←	7	7	1	4505.8773	-0.0018
9	8	1	←	8	7	1	5056.6073	-0.0021
9	7	2	←	8	6	2	5060.8725	-0.0022
9	6	3	←	8	5	3	5062.1615	0.0048
9	5	4	←	8	4	4	5062.2984	-0.0111
9	1	8	←	8	0	8	5062.5368	0.0151
9	9	0	←	8	8	0	5064.2544	-0.0044
9	9	1	←	8	8	1	5069.1409	0.0004
10	9	1	←	9	8	1	5618.5123	-0.0065

10	8	2	←	9	7	2	5622.7379	-0.0028
10	7	3	←	9	6	3	5624.4641	-0.0005
10	8	3	←	9	7	3	5624.5679	0.0174
10	6	4	←	9	5	4	5624.6781	-0.0002
10	3	7	←	9	2	7	5624.8923	0.0060
10	9	2	←	9	8	2	5625.2422	0.0018
10	10	0	←	9	9	0	5627.3360	-0.0003
10	10	1	←	9	9	1	5632.4073	-0.0009
11	10	1	←	10	9	1	6180.4436	-0.0089
11	9	2	←	10	8	2	6184.4758	-0.0071
11	8	3	←	10	7	3	6186.7129	-0.0066
11	7	4	←	10	6	4	6187.0111	-0.0010
11	5	6	←	10	4	6	6187.1994	-0.0046
11	4	7	←	10	3	7	6187.2868	0.0178
11	10	2	←	10	9	2	6187.7594	-0.0111
11	11	0	←	10	10	0	6190.5091	-0.0063
11	11	1	←	10	10	1	6195.6802	-0.0012
12	11	1	←	11	10	1	6742.4042	-0.0108
12	10	2	←	11	9	2	6746.0873	-0.0142
12	9	3	←	11	8	3	6748.9134	-0.0009
12	10	3	←	11	9	3	6749.1195	-0.0107
12	8	4	←	11	7	4	6749.3175	0.0102
12	7	5	←	11	6	5	6749.4502	-0.0005
12	6	6	←	11	5	6	6749.5538	0.0089
							RMS	**9.49 kHz**

Table S32. Assigned transitions for phenol trimer, 4-^{13}C isotopologue (para).

J'	K_a '	K_c '	←	J''	K_a''	K_c ''	ν_{obs} (MHz)	$\nu_{obs} - \nu_{calc}$
4	3	1	←	3	2	1	2241.2929	-0.0014
4	4	0	←	3	3	0	2246.2870	0.0036
5	4	1	←	4	3	1	2801.6855	0.0013
5	3	2	←	4	2	2	2806.5455	0.0042
5	5	0	←	4	4	0	2808.1704	0.0145
5	5	1	←	4	4	1	2813.3000	0.0081
6	5	1	←	5	4	1	3362.1239	0.0029
6	4	2	←	5	3	2	3367.4389	0.0005
6	3	3	←	5	2	3	3368.4872	-0.0066
6	2	4	←	5	1	4	3368.6120	0.0025
6	5	2	←	5	4	2	3368.9295	-0.0017
6	6	0	←	5	5	0	3370.2234	-0.0003
6	6	1	←	5	5	1	3376.0309	-0.0032
7	6	1	←	6	5	1	3922.6171	0.0001
7	5	2	←	6	4	2	3928.1247	-0.0003
7	4	3	←	6	3	3	3929.7747	-0.0006

7	5	3	←	6	4	3	3929.8356	-0.0026
7	3	4	←	6	2	4	3929.9633	-0.0004
7	2	5	←	6	1	5	3930.0396	-0.0027
7	6	2	←	6	5	2	3930.4880	-0.0035
7	7	0	←	6	6	0	3932.5238	0.0078
8	7	1	←	7	6	1	4483.1792	-0.0067
8	6	2	←	7	5	2	4488.5837	0.0000
8	5	3	←	7	4	3	4490.9772	-0.0106
8	6	3	←	7	5	3	4491.1126	-0.0007
8	4	4	←	7	3	4	4491.2826	0.0023
8	3	5	←	7	2	5	4491.3887	-0.0035
8	2	6	←	7	1	6	4491.4623	-0.0014
8	7	2	←	7	6	2	4492.0849	0.0000
8	8	0	←	7	7	0	4495.0551	0.0021
8	8	1	←	7	7	1	4501.6401	-0.0057
9	8	1	←	8	7	1	5043.8451	0.0020
9	7	2	←	8	6	2	5048.8067	-0.0029
9	6	3	←	8	5	3	5052.1175	0.0011
9	7	3	←	8	6	3	5052.3377	-0.0078
9	5	4	←	8	4	4	5052.5535	-0.0003
9	4	5	←	8	3	5	5052.7013	-0.0070
9	2	7	←	8	1	7	5052.8765	0.0019
9	1	8	←	8	0	8	5052.9346	-0.0017
9	8	2	←	8	7	2	5053.7091	-0.0066
9	9	0	←	8	8	0	5057.8397	-0.0020
9	9	1	←	8	8	1	5064.5191	-0.0015
10	9	1	←	9	8	1	5604.5984	-0.0079
10	8	2	←	9	7	2	5608.8123	-0.0010
10	7	3	←	9	6	3	5613.1443	0.0002
10	8	3	←	9	7	3	5613.5105	-0.0246
10	6	4	←	9	5	4	5613.7853	0.0070
10	5	5	←	9	4	5	5613.9855	-0.0007
10	4	6	←	9	3	6	5614.1057	-0.0039
10	3	7	←	9	2	7	5614.1992	-0.0004
10	2	8	←	9	1	8	5614.2772	0.0023
10	9	2	←	9	8	2	5615.3870	-0.0013
10	10	0	←	9	9	0	5620.8731	-0.0016
10	10	1	←	9	9	1	5627.4401	-0.0024
11	10	1	←	10	9	1	6165.4971	0.0023
11	9	2	←	10	8	2	6168.6117	-0.0096
11	8	3	←	10	7	3	6174.0478	-0.0042
11	9	3	←	10	8	3	6174.6524	-0.0311
11	7	4	←	10	6	4	6174.9585	0.0110
11	6	5	←	10	5	5	6175.2241	0.0022
11	5	6	←	10	4	6	6175.3821	0.0028
11	4	7	←	10	3	7	6175.4882	-0.0030

11	3	8	←	10	2	8	6175.5863	0.0041
11	2	9	←	10	1	9	6175.6688	0.0048
11	1	10	←	10	0	10	6175.7543	0.0121
11	10	2	←	10	9	2	6177.1377	0.0311
11	11	0	←	10	10	0	6184.1269	-0.0017
11	11	1	←	10	10	1	6190.4112	0.0010
12	11	1	←	11	10	1	6726.5236	-0.0063
12	10	2	←	11	9	2	6728.2882	0.0144
12	9	3	←	11	8	3	6734.8200	0.0005
12	10	3	←	11	9	3	6735.7808	-0.0130
12	9	4	←	11	8	4	6736.1026	0.0170
12	7	5	←	11	6	5	6736.4212	0.0104
12	6	6	←	11	5	6	6736.6070	-0.0018
12	5	7	←	11	4	7	6736.7584	0.0123
12	4	8	←	11	3	8	6736.8549	-0.0004
12	3	9	←	11	2	9	6736.9751	0.0240
12	2	10	←	11	1	10	6737.0584	0.0172
12	12	0	←	11	11	0	6747.5490	-0.0180
13	11	2	←	12	10	2	7287.8241	0.0040
13	10	3	←	12	9	3	7295.4059	-0.0186
13	11	3	←	12	10	3	7296.9023	0.0317
13	9	4	←	12	8	4	7297.1101	0.0169
13	8	5	←	12	7	5	7297.5419	-0.0068
13	7	6	←	12	6	6	7297.7766	-0.0176
13	6	7	←	12	5	7	7297.9621	0.0010
13	5	8	←	12	4	8	7298.1113	0.0203
13	4	9	←	12	3	9	7298.2054	0.0027
13	3	10	←	12	2	10	7298.3033	-0.0025
13	2	11	←	12	1	11	7298.4108	0.0049
13	12	2	←	12	11	2	7300.7025	0.0071
13	13	0	←	12	12	0	7311.1373	-0.0072
13	13	1	←	12	12	1	7316.4733	0.0017
14	11	3	←	13	10	3	7855.8313	-0.0130
14	9	5	←	13	8	5	7858.6265	-0.0047
14	8	6	←	13	7	6	7858.9217	-0.0102
14	7	7	←	13	6	7	7859.1234	-0.0094
14	6	8	←	13	5	8	7859.2734	-0.0127
14	5	9	←	13	4	9	7859.4145	-0.0010
14	3	11	←	13	2	11	7859.6272	-0.0185
14	2	12	←	13	1	12	7859.7414	-0.0159
14	13	2	←	13	12	2	7862.6041	0.0322
							RMS	**10.3 kHz**

Table S32. Assigned transitions for phenol trimer, 5-^{13}C isotopologue

J'	K_a '	K_c '	←	J''	K_a''	K_c ''	ν_{obs} (MHz)	$\nu_{obs} - \nu_{calc}$
4	3	1	←	3	2	1	2241.43262	0.00856
4	2	2	←	3	1	2	2246.28697	0.02615
4	1	3	←	3	0	3	2246.70099	0.00074
4	3	2	←	3	2	2	2246.86242	-0.00358
4	4	0	←	3	3	0	2247.4172	-0.00244
4	4	1	←	3	3	1	2252.45853	0.00866
5	4	1	←	4	3	1	2801.8825	0.00045
5	3	2	←	4	2	2	2807.42122	-0.0141
5	4	2	←	4	3	2	2808.63576	-0.00443
5	5	0	←	4	4	0	2809.70126	-0.00361
5	5	1	←	4	4	1	2815.65102	-0.00076
6	5	1	←	5	4	1	3362.40872	-0.00395
6	4	2	←	5	3	2	3368.35966	-0.00147
6	2	4	←	5	1	4	3369.99603	0.00333
6	5	2	←	5	4	2	3370.45458	0.00182
6	6	0	←	5	5	0	3372.26418	-0.0011
6	6	1	←	5	5	1	3378.91139	0.00256
7	5	2	←	6	4	2	3929.01224	0.00485
7	4	3	←	6	3	3	3931.29843	0.0069
7	5	3	←	6	4	3	3931.39835	0.00209
7	3	4	←	6	2	4	3931.55212	-0.00762
7	2	5	←	6	1	5	3931.66341	-0.0007
7	1	6	←	6	0	6	3931.73375	0.0034
7	6	2	←	6	5	2	3932.31125	0.00002
7	7	0	←	6	6	0	3935.12982	-0.00733
7	7	1	←	6	6	1	3942.2311	0.00337
8	7	1	←	7	6	1	4483.76298	-0.00811
8	6	2	←	7	5	2	4489.36772	0.0072
8	5	3	←	7	4	3	4492.65778	-0.00103
8	6	3	←	7	5	3	4492.87163	0.00404
8	4	4	←	7	3	4	4493.08049	-0.00041
8	1	7	←	7	0	7	4493.39792	0.00666
8	7	2	←	7	6	2	4494.2217	-0.00124
8	8	0	←	7	7	0	4498.33479	-0.00487
8	8	1	←	7	7	1	4505.61399	0.00098
9	8	1	←	8	7	1	5044.63155	-0.01369
9	7	2	←	8	6	2	5049.43413	0.00499
9	6	3	←	8	5	3	5053.91479	0.00425
9	7	3	←	8	6	3	5054.29145	-0.00006
9	5	4	←	8	4	4	5054.55369	0.00464
9	4	5	←	8	3	5	5054.76139	0.00206
9	3	6	←	8	2	6	5054.88362	0.00094
9	2	7	←	8	1	7	5054.9657	-0.00562

9	8	2	←	8	7	2	5056.19053	-0.00451
9	9	0	←	8	8	0	5061.86181	-0.0083
10	9	1	←	9	8	1	5605.67035	-0.01477
10	8	2	←	9	7	2	5609.24632	0.00021
10	7	3	←	9	6	3	5615.02231	0.00038
10	8	3	←	9	7	3	5615.66576	-0.00501
10	6	4	←	9	5	4	5615.96561	0.00896
10	5	5	←	9	4	5	5616.24205	-0.00056
10	4	6	←	9	3	6	5616.40171	-0.00321
10	3	7	←	9	2	7	5616.51322	-0.00506
10	2	8	←	9	1	8	5616.6118	0.00287
10	1	9	←	9	0	9	5616.68245	-0.00649
10	9	2	←	9	8	2	5618.23332	-0.00099
10	10	0	←	9	9	0	5625.69701	-0.00494
10	10	1	←	9	9	1	5632.59771	0.00846
11	10	1	←	10	9	1	6166.92562	0.0044
11	9	2	←	10	8	2	6168.8674	0.00122
11	8	3	←	10	7	3	6175.9632	-0.00218
11	9	3	←	10	8	3	6177.0053	-0.00508
11	7	4	←	10	6	4	6177.2839	-0.01158
11	6	5	←	10	5	5	6177.6803	0.00398
11	4	7	←	10	3	7	6178.0275	-0.00095
11	3	8	←	10	2	8	6178.1406	0.00086
11	1	10	←	10	0	10	6178.3147	-0.00964
11	10	2	←	10	9	2	6180.35672	0.00967
11	11	0	←	10	10	0	6189.7806	-0.00681
11	11	1	←	10	10	1	6196.15706	-0.02057
12	10	2	←	11	9	2	6728.3611	0.00199
12	10	3	←	11	9	3	6738.3178	0.0003
12	9	4	←	11	8	4	6738.611	-0.00602
12	7	5	←	11	6	5	6739.0498	-0.00562
12	6	6	←	11	5	6	6739.3163	-0.00452
12	5	7	←	11	4	7	6739.4952	-0.00297
12	4	8	←	11	3	8	6739.6096	-0.02381
12	3	9	←	11	2	9	6739.76561	0.01821
12	1	11	←	11	0	11	6739.96674	0.01696
12	11	2	←	11	10	2	6742.5401	0.00116
12	12	0	←	11	11	0	6754.0559	-0.00861
13	12	1	←	12	11	1	7290.12171	0.00785
13	11	3	←	12	10	3	7299.63695	0.03586
13	10	4	←	12	9	4	7299.84868	0.01207
13	8	5	←	12	7	5	7300.39829	0.02355
13	7	6	←	12	6	6	7300.6991	-0.00707
13	6	7	←	12	5	7	7300.95747	0.03371
13	5	8	←	12	4	8	7301.08639	-0.00017

13	4	9	←	12	3	9	7301.22292	0.00181
13	3	10	←	12	2	10	7301.35278	0.01173
13	2	11	←	12	1	11	7301.4587	0.00469
13	1	12	←	12	0	12	7301.55171	-0.0128
13	13	0	←	12	12	0	7318.49049	0.02389
13	13	1	←	12	12	1	7323.55557	0.0233
14	13	1	←	13	12	1	7852.14382	0.00741
14	11	3	←	13	10	3	7857.46836	-0.01945
14	10	4	←	13	9	4	7860.786	-0.01704
14	11	4	←	13	10	4	7860.9735	-0.01044
14	9	5	←	13	8	5	7861.6184	-0.01059
14	8	6	←	13	7	6	7862.03296	-0.00462
14	7	7	←	13	6	7	7862.32481	0.02324
14	6	8	←	13	5	8	7862.4819	-0.01393
14	5	9	←	13	4	9	7862.6347	-0.01889
14	4	10	←	13	3	10	7862.79803	0.00613
14	3	11	←	13	2	11	7862.9150	-0.00528
14	2	12	←	13	1	12	7863.0428	-0.00158
14	14	0	←	13	13	0	7882.92192	-0.00943
14	14	1	←	13	13	1	7887.26786	-0.01624
							RMS	**10.4 kHz**

Table S33. Assigned transitions for phenol trimer, 6-^{13}C isotopologue**.**

J'	K_a '	K_c '	←	J''	K_a''	K_c ''	ν_{obs} (MHz)	ν_{obs} - ν_{calc}
4	3	1	←	3	2	1	2246.4763	0.0022
4	4	0	←	3	3	0	2250.4614	0.0040
5	3	2	←	4	2	2	2812.2113	0.0022
5	2	3	←	4	1	3	2812.6006	-0.0141
5	4	2	←	4	3	2	2812.7805	0.0105
5	5	1	←	4	4	1	2817.5235	-0.0003
6	4	2	←	5	3	2	3374.3737	0.0026
6	2	4	←	5	1	4	3375.1448	-0.0011
6	5	2	←	5	4	2	3375.3498	0.0009
6	6	0	←	5	5	0	3376.1947	0.0009
6	6	1	←	5	5	1	3381.0698	-0.0048
7	6	1	←	6	5	1	3931.5521	0.0275
7	5	2	←	6	4	2	3936.3887	0.0023
7	6	2	←	6	5	2	3937.9441	0.0029
7	7	0	←	6	6	0	3939.2678	-0.0023
7	7	1	←	6	6	1	3944.6473	-0.0008
8	7	1	←	7	6	1	4493.2938	0.0151
8	6	2	←	7	5	2	4498.2418	0.0033
8	3	5	←	7	2	5	4500.1111	-0.0020
8	7	2	←	7	6	2	4500.5486	-0.0007

8	8	0	←	7	7	0	4502.5069	-0.0017
8	8	1	←	7	7	1	4508.2461	0.0000
9	8	1	←	8	7	1	5055.0707	-0.0104
9	7	2	←	8	6	2	5059.9224	0.0054
9	6	3	←	8	5	3	5062.1615	0.0109
9	4	5	←	8	3	5	5062.5347	-0.0008
9	3	6	←	8	2	6	5062.6115	0.0048
9	8	2	←	8	7	2	5063.1787	0.0037
9	9	0	←	8	8	0	5065.9233	0.0038
9	9	1	←	8	8	1	5071.8658	-0.0041
10	9	1	←	9	8	1	5616.9392	-0.0024
10	8	2	←	9	7	2	5621.4211	0.0018
10	7	3	←	9	6	3	5624.3881	0.0016
10	8	3	←	9	7	3	5624.5679	-0.0251
10	5	5	←	9	4	5	5624.9113	-0.0141
10	3	7	←	9	2	7	5625.0874	0.0002
10	2	8	←	9	1	8	5625.1559	0.0053
10	9	2	←	9	8	2	5625.8236	0.0030
10	10	0	←	9	9	0	5629.5031	-0.0024
10	10	1	←	9	9	1	5635.5163	-0.0033
11	10	1	←	10	9	1	6178.8702	-0.0002
11	9	2	←	10	8	2	6182.7505	-0.0015
11	8	3	←	10	7	3	6186.5408	-0.0001
11	7	4	←	10	6	4	6187.0871	-0.0061
11	6	5	←	10	5	5	6187.2868	0.0074
11	5	6	←	10	4	6	6187.3957	0.0022
11	3	8	←	10	2	8	6187.5617	0.0067
11	2	9	←	10	1	9	6187.6312	0.0052
11	10	2	←	10	9	2	6188.4893	0.0013
11	11	0	←	10	10	0	6193.2611	0.0009
11	11	1	←	10	10	1	6199.1959	0.0015
12	11	1	←	11	10	1	6740.8707	-0.0088
12	10	2	←	11	9	2	6743.9259	-0.0049
12	9	3	←	11	8	3	6748.5952	-0.0058
12	10	3	←	11	9	3	6749.1195	0.0015
12	5	7	←	11	4	7	6749.8369	-0.0027
12	4	8	←	11	3	8	6749.9285	0.0007
12	2	10	←	11	1	10	6750.0887	-0.0013
12	1	11	←	11	0	11	6750.1734	0.0017
12	11	2	←	11	10	2	6751.1814	0.0025
12	12	0	←	11	11	0	6757.1680	-0.0002
12	12	1	←	11	11	1	6762.8953	0.0024
13	11	2	←	12	10	2	7304.9709	-0.0090
13	10	3	←	12	9	3	7310.5462	-0.0065
13	11	3	←	12	10	3	7311.3329	0.0101
13	9	4	←	12	8	4	7311.5523	-0.0115

13	8	5	←	12	7	5	7311.8577	-0.0072
13	6	7	←	12	5	7	7312.1647	0.0017
13	5	8	←	12	4	8	7312.2633	-0.0029
13	4	9	←	12	3	9	7312.3598	-0.0002
13	3	10	←	12	2	10	7312.4537	0.0030
13	2	11	←	12	1	11	7312.5425	0.0007
13	12	2	←	12	11	2	7313.8989	0.0040
13	13	0	←	12	12	0	7321.2067	0.0008
13	13	1	←	12	12	1	7326.6227	0.0101
14	13	1	←	13	12	1	7865.1832	-0.0068
14	12	2	←	13	11	2	7865.9499	0.0204
14	11	3	←	13	10	3	7872.3624	-0.0185
14	12	3	←	13	11	3	7873.4998	0.0087
14	11	4	←	13	10	4	7873.7523	0.0003
14	8	6	←	13	7	6	7874.3008	0.0016
14	6	8	←	13	5	8	7874.5655	-0.0017
14	5	9	←	13	4	9	7874.6698	-0.0044
14	4	10	←	13	3	10	7874.7764	0.0003
14	13	2	←	13	12	2	7876.6387	0.0014
14	14	0	←	13	13	0	7885.3433	-0.0007
14	14	1	←	13	13	1	7890.3490	-0.0011
							RMS	**7.11 kHz**

Table S34. Unscaled harmonic frequencies for the phenol dimer, calculated at the M06-2X/6-311++g(d,p) level of theory. Versanyi normal mode notation is used to describe most of the vibrations, noted as "Xa/b-type" in the description, where X is the normal mode # used by Versanyi[5].

Mode	ν (cm^{-1})	Description
ν_1	27.82	"Hinge"
ν_2	46.97	Intermolecular torsions
ν_3	49.65	"
ν_4	87.27	"
ν_5	94.00	"
ν_6	132.64	"
ν_7	242.85	Hinge + donor ring deform.
ν_8	246.20	Hinge + acceptor ring deform.
ν_9	393.37	acceptor O-H torsion
ν_{10}	421.21	in-phase donor/acceptor O-H rock
ν_{11}	424.09	in-phase intermolecular ring twist
ν_{12}	425.97	out of phase intermol. Ring twist
ν_{13}	442.97	out of phase donor/accept O-H rock
ν_{14}	521.53	in-phase intermol. ring wag
ν_{15}	527.95	donor ring butterfly
ν_{16}	536.54	6a-type, acceptor
ν_{17}	538.49	6a-type, donor
ν_{18}	627.44	6b-type, acceptor
ν_{19}	631.12	6b-type, donor
ν_{20}	695.46	donor O-H torsion
ν_{21}	707.28	11-type, acceptor
ν_{22}	713.06	11-type, donor
ν_{23}	779.73	11-type, intermol., in-phase
ν_{24}	782.80	11-type, intermol., out of phase
ν_{25}	834.29	12-type, acceptor
ν_{26}	840.79	12-type, donor
ν_{27}	851.91	10a-type, acceptor
ν_{28}	856.33	10a-type, donor
ν_{29}	917.75	10b-type, donor
ν_{30}	924.99	10b-type, acceptor
ν_{31}	992.41	16b-type, donor
ν_{32}	996.87	16b-type, acceptor
ν_{33}	1007.29	4-type, donor
ν_{34}	1014.87	12-type, donor

[5] Versanyi, G. *Assignments for Vibrational Spectra of Seven Hundred Benzene Derivatives*, vol 1-2; Academic Press: Budapest, New York, 1974.

ν_{35}	1015.72	12-type, acceptor
ν_{36}	1019.40	4-type, acceptor
ν_{37}	1056.77	16a-type, acceptor
ν_{38}	1060.20	16a-type, donor
ν_{39}	1105.92	18b-type, acceptor
ν_{40}	1109.78	18b-type, donor
ν_{41}	1169.64	14-type, acceptor
ν_{42}	1174.02	14-type, donor
ν_{43}	1192.10	9a-type, acceptor
ν_{44}	1195.16	9a-type, donor
ν_{45}	1217.68	9b-type, acceptor
ν_{46}	1251.35	9b-type, donor
ν_{47}	1288.53	18a-type, acceptor
ν_{48}	1313.84	18a-type, donor
ν_{49}	1339.37	8b-type, acceptor
ν_{50}	1347.88	8b-type, donor
ν_{51}	1368.79	3-type, acceptor
ν_{52}	1394.58	3-type, donor
ν_{53}	1514.81	14-type, acceptor
ν_{54}	1520.66	14-type, donor
ν_{55}	1540.26	19a-type, acceptor
ν_{56}	1552.86	19a-type, donor
ν_{57}	1670.11	15-type, donor
ν_{58}	1676.28	15-type, acceptor
ν_{59}	1679.67	14-type, acceptor
ν_{60}	1687.73	14-type, donor
ν_{61}	3158.10	13-type, acceptor
ν_{62}	3168.94	20a-type, donor
ν_{63}	3174.85	13-type, donor
ν_{64}	3176.03	20a-type, acceptor (out of phase)
ν_{65}	3184.19	20b-type, acceptor (out of phase)
ν_{66}	3184.75	20b-type, donor
ν_{67}	3191.41	20b-type, acceptor (opposite phase as 65)
ν_{68}	3197.70	20b-type, donor (opposite phase as 66)
ν_{69}	3200.61	20a-type, acceptor (in phase)
ν_{70}	3206.40	20a-type, donor (in phase)
ν_{71}	3728.02	O-H stretch, donor
ν_{72}	3871.03	O-H stretch, acceptor

Table S35. Unscaled harmonic frequencies for the phenol trimer, calculated at the M06-2X/6-311++g(d,p) level of theory.

Mode	ν (cm^{-1})	Mode	ν (cm^{-1})
$\nu_{1\,E}$	20.68	$\nu_{20\,A}$	1014.51
$\nu_{1\,A}$	27.34	$\nu_{20\,E}$	1015.18
$\nu_{2\,E}$	32.10	$\nu_{21\,E}$	1056.79
$\nu_{2\,A}$	42.77	$\nu_{21\,A}$	1057.46
$\nu_{3\,E}$	59.59	$\nu_{22\,E}$	1106.66
$\nu_{3\,A}$	76.95	$\nu_{22\,A}$	1108.19
$\nu_{4\,E}$	133.28	$\nu_{23\,E}$	1172.38
$\nu_{4\,A}$	163.88	$\nu_{23\,A}$	1173.19
$\nu_{5\,E}$	249.79	$\nu_{24\,A}$	1192.48
$\nu_{5\,A}$	265.58	$\nu_{24\,E}$	1192.65
$\nu_{6\,E}$	418.10	$\nu_{25\,E}$	1228.04
$\nu_{6\,A}$	419.42	$\nu_{25\,A}$	1274.19
$\nu_{7\,E}$	428.93	$\nu_{26\,E}$	1303.38
$\nu_{7\,A}$	441.12	$\nu_{26\,A}$	1316.24
$\nu_{8\,A}$	520.07	$\nu_{27\,E}$	1353.57
$\nu_{8\,E}$	522.00	$\nu_{27\,A}$	1353.62
$\nu_{9\,E}$	537.24	$\nu_{28\,E}$	1371.59
$\nu_{9\,A}$	541.23	$\nu_{28\,A}$	1400.64
ν_{10}	588.29	$\nu_{29\,E}$	1514.57
$\nu_{11\,A}$	627.13	$\nu_{29\,A}$	1520.56
$\nu_{11\,E}$	627.86	$\nu_{30\,E}$	1547.20
$\nu_{12\,A}$	701.17	$\nu_{30\,A}$	1552.22
$\nu_{12\,E}$	705.48	$\nu_{31\,E}$	1676.83
$\nu_{13\,E}$	776.83	$\nu_{31\,A}$	1681.86
$\nu_{13\,A}$	778.04	$\nu_{32\,E}$	1686.93
$\nu_{14\,A}$	836.52	$\nu_{32\,A}$	1691.29
$\nu_{14\,E}$	838.53	$\nu_{33\,E}$	3211.59
$\nu_{15\,A}$	847.64	$\nu_{33\,A}$	3211.95
$\nu_{15\,E}$	848.84	$\nu_{34\,E}$	3217.71
ν_{16}	903.04	$\nu_{34\,A}$	3217.94
$\nu_{17\,A}$	917.73	$\nu_{35\,E}$	3225.82
$\nu_{17\,E}$	918.90	$\nu_{35\,A}$	3228.98
$\nu_{18\,E}$	992.44	$\nu_{36\,E}$	3223.96
$\nu_{18\,A}$	993.99	$\nu_{36\,A}$	3233.97
$\nu_{19\,A}$	1010.34	$\nu_{37\,E}$	3241.80
$\nu_{19\,E}$	1010.71	$\nu_{37\,A}$	3242.02
		$\nu_{38\,A}$	3664.19
		$\nu_{38\,E}$	3707.46