Supplementary Material: Structural locking mediated by a water wire: a high-resolution rotational spectroscopy study on hydrated forms of a chiral biphenyl derivative

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Contents

1 Experimental methods

The sample was purchased from Sigma-Aldrich (96%) and used without further purification. To create sufficient vapour pressure the sample was heated to 50°C directly at the nozzle. Further experimental details can be found in reference 18 of the main article.

2 Molecular structure

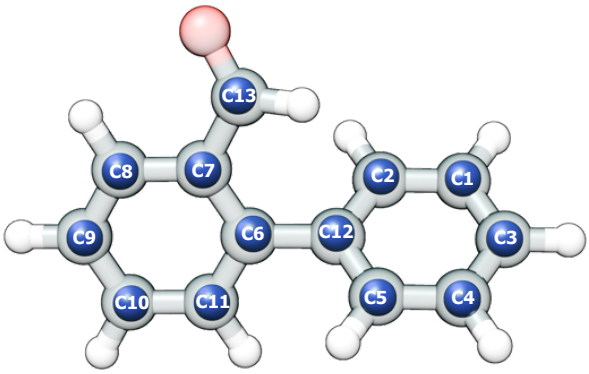

Figure 1: Carbon atom labelling of free biphenyl-2-carboxaldehyde (BPCO).

3 Rotational constants of the ^{13}C isotopologues

Table 1: Rotational constants for singly substituted ^{13}C isotopologues of biphenyl-carboxaldehyde (BPCO). The errors given here for the measured values are standard errors. N is the number of lines included in the fit and σ is the standard deviation of the fit. The centrifugal distortion constants were kept fixed to the values of the free BPCO (see main paper).

	A/MHz	B/MHz	C/MHz	N	σ/kHz
C1	1230.78795(32)	496.35936(23)	383.62365(11)	24	4.6
C2	1231.24738(41)	500.05742(21)	385.95986(11)	26	4.9
C3	1234.88492(34)	494.75244(25)	382.65325(12)	15	3.9
C4	1230.46110(62)	496.96842(42)	384.05070(19)	14	6.2
C5	1229.67970(32)	499.73767(27)	385.53602(15)	16	4.8
C6	1234.08984(49)	501.59758(31)	386.66462(17)	18	6.6
C7	1234.11717(37)	500.70307(21)	386.13360(10)	17	3.7
C8	1234.72414(67)	497.84910(58)	384.48921(18)	15	6.9
C9	1231.62206(31)	496.46676(42)	383.37861(10)	17	4.1
C10	1221.77508(50)	498.95250(53)	383.91481(15)	19	5.9
C11	1224.74825(50)	501.21736(29)	385.52989(21)	16	5.1
C12	1234.64325(44)	501.23734(26)	386.50349(14)	16	5.0
C13	1223.56033(58)	501.13705(34)	385.42501(18)	17	5.9

4 Rotational constants of BPCO-1w(I)-^{18}O

Table 2: Rotational constants for BPCO-1w(I)-^{16}O and BPCO-1w(I)-^{18}O. The errors given here for the measured values are standard errors. N is the number of lines included in the fit and σ is the standard deviation of the fit. The centrifugal distortion constants of BPCO-1w(I)-^{18}O were kept fixed to the values of BPCO-1w(I)-^{16}O (see main paper).

	BPCO-1w(I)-^{16}O	BPCO-1w(I)-^{18}O
A/MHz	974.76725(54)	965.1307(12)
B/MHz	358.03677(13)	346.73718(16)
C/MHz	278.11019(11)	270.49545(11)
N	125	69
σ/kHz	5.4	8.9

5 Rotational constants of BPCO-1w(II)-^{18}O

Table 3: Rotational constants for BPCO-1w(II)-^{16}O and BPCO-1w(II)-^{18}O. The errors given here for the measured values are standard errors. N is the number of lines included in the fit and σ is the standard deviation of the fit. The centrifugal distortion constants of BPCO-1w(II)-^{18}O were kept fixed to the values of BPCO-1w(II)-^{16}O (see main paper).

	BPCO-1w(II)-^{16}O	BPCO-1w(II)-^{18}O
A/MHz	627.43661(55)	599.0369(11)
B/MHz	498.72577(28)	498.09483(66)
C/MHz	296.54810(27)	289.88841(64)
N	65	44
σ/kHz	8.7	13.6

6 Rotational constants of BPCO-2w(II)-^{16}O(1)-^{18}O(2) and BPCO-2w(II)-^{18}O(1)-^{16}O(2)

Table 4: Rotational constants for BPCO-2w(II)-^{16}O(1)-^{18}O(2) and BPCO-2w(II)-^{18}O(1)-^{16}O(2). The errors given here for the measured values are standard errors. N is the number of lines included in the fit and σ is the standard deviation of the fit. The centrifugal distortion constants were kept fixed to the values of BPCO-2w(II) (see main paper).

	BPCO-2w(II)-^{16}O(1)-^{16}O(2)	BPCO-2w(II)-^{18}O(1)-^{16}O(2)	BPCO-2w(II)-^{16}O(1)-^{18}O(2)
A/MHz	496.65614(61)	492.77645(92)	487.25957(74)
B/MHz	437.48228(30)	428.61414(31)	430.61451(32)
C/MHz	258.28601(21)	255.24197(18)	253.59915(12)
N	37	14	13
σ/kHz	2.8	4.7	4.1

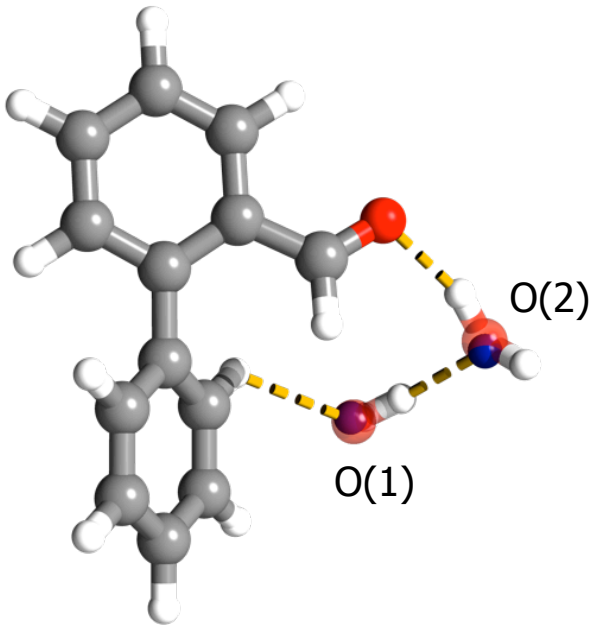

Figure 2: Molecular structure of BPCO-2w(II) with labelled oxygens.

7 Kraitchman calculations

7.1 Free BPCO

Table 5: Calculated (B3LYP-D3) carbon atom coordinates in the principal axis frame.

	X	Y	Z
C1	-2.946678	0.820676	0.910261
C2	-1.570702	0.631923	0.896795
C3	-3.760789	0.088137	0.053620
C4	-3.190104	-0.838053	-0.812729
C5	-1.814626	-1.029866	-0.822781
C6	0.481298	-0.525374	0.030671
C7	1.421995	0.516238	-0.091896
C8	2.790285	0.236003	-0.007094
C9	3.239757	-1.059078	0.175077
C10	2.315091	-2.096789	0.270933
C11	0.955921	-1.829882	0.201132
C12	-0.984127	-0.292577	0.026787
C13	1.018633	1.909338	-0.404217

Table 6: Carbon atom coordinates obtained from the Kraitchman calculation.

	X	Y	Z
C1	-3.18353	-0.82563	-0.84161
C2	-1.56822	0.61134	0.92028
C3	-3.76387	0.08757	0.00000
C4	-2.95332	0.79041	0.93409
C5	-1.79956	-1.01821	-0.84446
C6	0.43189	-0.50952	0.10202
C7	1.41190	0.50491	-0.08256
C8	2.79248	0.24421	0.01220
C9	3.25367	-1.04182	0.16122
C10	2.33384	-2.09312	0.25537
C11	0.96308	-1.83686	0.17684
C12	-0.95644	-0.27934	0.08930
C13	0.99204	1.91595	-0.36991

7.2 BPCO-1w(I)

Table 7: Calculated (B3LYP-D3) vs Kraitchman atom coordinates for the oxygen atom of water in BPCO-1w(I).

	X	Y	Z
Calculated			
O	-4.711214	1.656407	-0.141108
Kraitchman			
O	-4.80001	1.65496	-0.06855

7.3 BPCO-1w(II)

Table 8: Calculated (B3LYP-D3) vs Kraitchman atom coordinates for the oxygen atom of water in BPCO-1w(II).

	X	Y	Z
Calculated			
O	-0.296457	4.498623	-0.306561
Kraitchman			
O	-0.68010	4.38889	-0.29203

7.4 BPCO-2w(II)

Table 9: Calculated (B3LYP-D3) vs Kraitchman atom coordinates for oxygen atoms of water molecules in BPCO-2w(II).

	X	Y	Z
Calculated			
O1	3.148924	-1.438928	1.388300
O2	2.650065	-3.375244	-0.601630
Kraitchman			
O1	3.09264	-1.45961	1.48817
O2	2.75679	-3.25403	-0.70328

8 Appendix A: Line lists

8.1 BPCO

Table 10: Observed and calculated rotational transitions (MHz) for free BPCO.

Observed	Calculated	Obs-Calc	J′	K_a′	K_c′	J″	K_a″	K_c″
2001.8231	2001.8246	-0.0015	4	2	2	4	1	3
2019.4194	2019.4192	0.0002	6	2	4	6	1	5
2096.9507	2096.9513	-0.0006	3	2	1	3	1	2
2189.7177	2189.7163	0.0014	7	2	5	7	1	6
2212.0859	2212.0875	-0.0016	2	2	0	2	1	1
2395.2759	2395.2848	-0.0089	2	1	2	1	0	1
2485.7030	2485.7056	-0.0026	3	1	3	2	1	2
2493.6110	2493.6106	0.0004	8	2	6	8	1	7
2498.9061	2498.9082	-0.0021	6	1	5	6	0	6
2544.3133	2544.3122	0.0011	2	2	1	2	1	2
2616.5210	2616.5211	-0.0001	3	0	3	2	0	2
2665.4678	2665.4669	0.0009	3	2	2	2	2	1
2714.4181	2714.4152	0.0029	3	2	1	2	2	0
2724.0655	2724.0735	-0.0080	3	2	2	3	1	3
2829.5531	2829.5514	0.0017	3	1	2	2	1	1
2842.1507	2842.1492	0.0015	5	1	4	4	2	3
2937.2098	2937.2079	0.0019	4	0	4	3	1	3
2938.9356	2938.9347	0.0009	9	2	7	9	1	8
2966.7280	2966.7306	-0.0026	4	2	3	4	1	4
3002.9056	3002.9019	0.0037	9	3	6	9	2	7
3116.4845	3116.4843	0.0002	3	1	3	2	0	2
3117.9279	3117.9301	-0.0022	8	3	5	8	2	6
3142.1037	3142.1015	0.0022	7	2	5	6	3	4
3144.7458	3144.7494	-0.0036	7	1	6	7	0	7
3272.6994	3272.6960	0.0034	5	2	4	5	1	5
3301.5733	3301.5679	0.0054	4	1	4	3	1	3
3437.1687	3437.1711	-0.0024	4	0	4	3	0	3
3503.5475	3503.5489	-0.0014	6	3	3	6	2	4
3544.2251	3544.2250	0.0001	4	2	3	3	2	2
3576.5430	3576.5413	0.0017	4	3	2	3	3	1

3581.6180	3581.6159	0.0021	4	3	1	3	3	0
3640.4113	3640.4138	-0.0025	6	2	5	6	1	6
3660.9662	3660.9638	0.0024	4	2	2	3	2	1
3686.2795	3686.2771	0.0024	5	3	2	5	2	3
3756.0905	3756.0904	0.0001	4	1	3	3	1	2
3801.5248	3801.5311	-0.0063	4	1	4	3	0	3
3820.7668	3820.7672	-0.0004	4	3	1	4	2	2
3847.7219	3847.7186	0.0033	8	1	7	8	0	8
3863.4060	3863.4038	0.0022	5	0	5	4	1	4
3960.6812	3960.6848	-0.0036	3	3	1	3	2	2
3993.0005	3993.0011	-0.0006	4	3	2	4	2	3
4055.3444	4055.3425	0.0019	5	3	3	5	2	4
4065.8721	4065.8752	-0.0031	7	2	6	7	1	7
4091.4912	4091.4928	-0.0016	2	2	1	1	1	0
4108.7898	4108.7860	0.0038	5	1	5	4	1	4
4158.3553	4158.3567	-0.0014	6	3	4	6	2	5
4218.8672	4218.8661	0.0011	2	2	0	1	1	1
4227.7663	4227.7639	0.0024	5	0	5	4	0	4
4311.5369	4311.5367	0.0002	7	3	5	7	2	6
4414.7568	4414.7515	0.0053	5	2	4	4	2	3
4473.1389	4473.1460	-0.0071	5	1	5	4	0	4
4477.0887	4477.0928	-0.0041	5	3	3	4	3	2
4494.5614	4494.5592	0.0022	5	3	2	4	3	1
4522.2328	4522.2322	0.0006	8	3	6	8	2	7
4542.7091	4542.7028	0.0063	8	2	7	8	1	8
4571.6984	4571.6927	0.0057	9	1	8	9	0	9
4629.0532	4629.0493	0.0039	5	2	3	4	2	2
4665.8159	4665.8128	0.0031	5	1	4	4	1	3
4752.9643	4752.9611	0.0032	6	0	6	5	1	5
4865.0755	4865.0806	-0.0051	3	2	2	2	1	1
4907.5393	4907.5400	-0.0007	6	1	6	5	1	5
4997.1979	4997.1933	0.0046	9	4	5	9	3	6
4998.3507	4998.3433	0.0074	6	0	6	5	0	5
5062.7841	5062.7888	-0.0047	9	2	8	9	1	9
5110.7499	5110.7419	0.0080	7	1	6	6	2	5
5130.8898	5130.8876	0.0022	10	3	8	10	2	9

5152.9222	5152.9222	0.0000	6	1	6	5	0	5
5203.2080	5203.1989	0.0091	8	4	4	8	3	5
5271.1952	5271.2012	-0.0060	3	2	1	2	1	2
5275.2609	5275.2578	0.0031	6	2	5	5	2	4
5290.0778	5290.0802	-0.0024	10	1	9	10	0	10
5346.7781	5346.7838	-0.0057	7	4	3	7	3	4
5372.7773	5372.7895	-0.0122	6	4	3	5	4	2
5374.4987	5374.5026	-0.0039	6	4	2	5	4	1
5378.2725	5378.2720	0.0005	6	3	4	5	3	3
5423.4071	5423.4055	0.0016	6	3	3	5	3	2
5435.4730	5435.4653	0.0077	6	4	2	6	3	3
5484.3741	5484.3682	0.0059	5	4	1	5	3	2
5501.8478	5501.8467	0.0011	6	4	3	6	3	4
5503.7246	5503.7266	-0.0020	7	4	4	7	3	5
5507.3289	5507.3292	-0.0003	5	4	2	5	3	3
5508.4273	5508.4242	0.0031	4	4	0	4	3	1
5514.2943	5514.3029	-0.0086	4	4	1	4	3	2
5521.4713	5521.4633	0.0080	8	4	5	8	3	6
5551.7743	5551.7755	-0.0012	6	1	5	5	1	4
5565.4361	5565.4368	-0.0007	9	4	6	9	3	7
5579.7478	5579.7541	-0.0063	4	2	3	3	1	2
5606.1336	5606.1337	-0.0001	6	2	4	5	2	3
5606.4075	5606.4063	0.0012	7	0	7	6	1	6
5617.2758	5617.2743	0.0015	10	2	9	10	1	10
5646.7457	5646.7439	0.0018	10	4	7	10	3	8
5681.2115	5681.2092	0.0023	9	2	7	8	3	6
5698.8479	5698.8556	-0.0077	7	1	7	6	1	6
5853.4346	5853.4346	0.0000	7	1	7	6	0	6
6124.3200	6124.3170	0.0030	7	2	6	6	2	5
6212.8878	6212.8857	0.0021	8	1	7	7	2	6
6238.4193	6238.4152	0.0041	5	2	4	4	1	3
6254.4712	6254.4774	-0.0062	7	6	1	6	6	0
6254.4712	6254.4760	-0.0048	7	6	2	6	6	1
6263.8543	6263.8566	-0.0023	7	5	3	6	5	2
6263.9843	6263.9910	-0.0067	7	5	2	6	5	1
6277.4942	6277.4971	-0.0029	7	3	5	6	3	4

6279.3738	6279.3770	-0.0032	7	4	4	6	4	3
6285.0030	6285.0014	0.0016	7	4	3	6	4	2
6373.6835	6373.6829	0.0006	7	3	4	6	3	3
6406.8248	6406.8265	-0.0017	7	1	6	6	1	5
6431.0418	6431.0422	-0.0004	8	0	8	7	1	7
6446.4590	6446.4594	-0.0004	4	2	2	3	1	3
6484.2271	6484.2298	-0.0027	8	1	8	7	1	7
6523.4973	6523.4916	0.0057	8	0	8	7	0	7
6576.6835	6576.6791	0.0044	8	1	8	7	0	7
6577.1274	6577.1235	0.0039	7	2	5	6	2	4
6613.6840	6613.6778	0.0062	3	3	1	2	2	0
6627.0092	6627.0041	0.0051	3	3	0	2	2	1
6847.8709	6847.8601	0.0108	6	2	5	5	1	4
6873.8794	6873.8762	0.0032	10	5	5	10	4	6
6946.4225	6946.4226	-0.0001	4	2	2	3	0	3
6961.0500	6961.0574	-0.0074	8	2	7	7	2	6
6964.5028	6964.5043	-0.0015	9	5	4	9	4	5
6996.4433	6996.4447	-0.0014	10	5	6	10	4	7
7019.9369	7019.9377	-0.0008	9	5	5	9	4	6
7021.5426	7021.5442	-0.0016	8	5	3	8	4	4
7043.7158	7043.7226	-0.0068	8	5	4	8	4	5
7056.5459	7056.5453	0.0006	7	5	2	7	4	3
7064.1553	7064.1537	0.0016	7	5	3	7	4	4
7077.5610	7077.5556	0.0054	6	5	1	6	4	2
7079.6604	7079.6741	-0.0137	6	5	2	6	4	3
7089.7935	7089.7895	0.0040	5	5	0	5	4	1
7155.1651	7155.1613	0.0038	8	6	2	7	6	1
7155.1651	7155.1521	0.0130	8	6	3	7	6	2
7169.0534	7169.0584	-0.0050	8	5	4	7	5	3
7169.5857	7169.5910	-0.0053	8	5	3	7	5	2
7171.7509	7171.7529	-0.0020	8	3	6	7	3	5
7189.4842	7189.4895	-0.0053	8	4	5	7	4	4
7204.5891	7204.5921	-0.0030	8	4	4	7	4	3
7226.4575	7226.4608	-0.0033	8	1	7	7	1	6
7235.5207	7235.5168	0.0039	9	0	9	8	1	8
7264.5043	7264.5067	-0.0024	9	1	8	8	2	7

7265.2328	7265.2420	-0.0092	9	1	9	8	1	8
7288.7026	7288.7043	-0.0017	9	0	9	8	0	8
7318.4388	7318.4295	0.0093	9	1	9	8	0	8
7348.1827	7348.1770	0.0057	8	3	5	7	3	4
7420.4023	7420.4015	0.0008	7	2	6	6	1	5
7475.8018	7475.8039	-0.0021	4	3	2	3	2	1
7530.3459	7530.3551	-0.0092	8	2	6	7	2	5
7543.1495	7543.1531	-0.0036	4	3	1	3	2	2
7773.9396	7773.9408	-0.0012	5	2	3	4	1	4
7785.3328	7785.3280	0.0048	9	2	8	8	2	7
7974.6343	7974.6325	0.0018	8	2	7	7	1	6

8.2 ^{13}C isotopologues of BPCO

Table 11: Observed and calculated rotational transitions (MHz) for singly substituted $^{13}C(1)$.

Observed	Calculated	Obs-Calc	J′	K_a'	K_c'	J″	K_a''	K_c''
3097.4006	3097.4018	-0.0012	3	1	3	2	0	2
4443.2997	4443.2920	0.0077	5	1	5	4	0	4
4580.5405	4580.5508	-0.0103	5	2	3	4	2	2
4706.1978	4706.2000	-0.0022	6	0	6	5	1	5
4843.2352	4843.2307	0.0045	3	2	2	2	1	1
5116.6351	5116.6369	-0.0018	6	1	6	5	0	5
5226.2778	5226.2777	0.0001	6	2	5	5	2	4
5240.5991	5240.5980	0.0011	3	2	1	2	1	2
5499.2750	5499.2727	0.0023	6	1	5	5	1	4
5510.4466	5510.4524	-0.0058	4	4	0	4	3	1
5547.3425	5547.3400	0.0025	6	2	4	5	2	3
5552.6874	5552.6895	-0.0021	4	2	3	3	1	2
5810.0436	5810.0349	0.0087	7	1	7	6	0	6
6207.1228	6207.1192	0.0036	5	2	4	4	1	3
6374.0698	6374.0745	-0.0047	8	0	8	7	1	7
6400.1003	6400.0962	0.0041	4	2	2	3	1	3
6589.0624	6589.0605	0.0019	3	3	1	2	2	0

6601.8747	6601.8734	0.0013	3	3	0	2	2	1
6812.9690	6812.9727	-0.0037	6	2	5	5	1	4
7173.2319	7173.2297	0.0022	9	0	9	8	1	8
7381.9497	7381.9517	-0.0020	7	2	6	6	1	5
7443.6667	7443.6704	-0.0037	4	3	2	3	2	1
7508.4329	7508.4296	0.0033	4	3	1	3	2	2
7959.1471	7959.1516	-0.0045	10	0	10	9	1	9

Table 12: Observed and calculated rotational transitions (MHz) for singly substituted $^{13}C(2)$.

Observed	Calculated	Obs-Calc	J′	K_a'	K_c'	J″	K_a''	K_c''
3792.8823	3792.8911	-0.0088	4	1	4	3	0	3
3853.1260	3853.1220	0.0040	5	0	5	4	1	4
4206.1379	4206.1359	0.0020	2	2	0	1	1	1
4740.8110	4740.8110	-0.0000	6	0	6	5	1	5
5254.6716	5254.6712	0.0004	3	2	1	2	1	2
5261.0157	5261.0218	-0.0061	6	2	5	5	2	4
5362.9866	5362.9919	-0.0053	6	3	4	5	3	3
5407.4833	5407.4786	0.0047	6	3	3	5	3	2
5565.0351	5565.0358	-0.0007	4	2	3	3	1	2
5588.8416	5588.8435	-0.0019	6	2	4	5	2	3
5747.6748	5747.6773	-0.0025	7	0	7	6	0	6
5840.5823	5840.5820	0.0003	7	1	7	6	0	6
6108.0175	6108.0256	-0.0081	7	2	6	6	2	5
6222.8305	6222.8174	0.0131	5	2	4	4	1	3
6354.5589	6354.5499	0.0090	7	3	4	6	3	3
6415.6560	6415.6567	-0.0007	8	0	8	7	1	7
6562.0933	6562.0989	-0.0056	8	1	8	7	0	7
6594.2391	6594.2359	0.0032	3	3	1	2	2	0
6607.4116	6607.4140	-0.0024	3	3	0	2	2	1
6831.6590	6831.6660	-0.0070	6	2	5	5	1	4
7218.5736	7218.5740	-0.0004	9	0	9	8	1	8
7302.0838	7302.0810	0.0028	9	1	9	8	0	8
7403.7427	7403.7284	0.0143	7	2	6	6	1	5

7454.1736	7454.1768	-0.0032	4	3	2	3	2	1
7520.7798	7520.7784	0.0014	4	3	1	3	2	2
7746.4191	7746.4212	-0.0021	5	2	3	4	1	4

Table 13: Observed and calculated rotational transitions (MHz) for singly substituted $^{13}C(3)$.

Observed	Calculated	Obs-Calc	J′	K_a'	K_c'	J″	K_a''	K_c''
3806.2525	3806.2527	-0.0002	5	0	5	4	1	4
4211.1965	4211.1988	-0.0023	2	2	0	1	1	1
5109.6155	5109.6201	-0.0046	6	1	6	5	0	5
5247.0297	5247.0321	-0.0024	3	2	1	2	1	2
5528.6899	5528.6914	-0.0015	6	2	4	5	2	3
5537.2783	5537.2799	-0.0016	7	0	7	6	1	6
5560.4678	5560.4667	0.0011	4	2	3	3	1	2
5636.4578	5636.4515	0.0063	7	1	7	6	1	6
6401.1962	6401.1920	0.0042	4	2	2	3	1	3
6608.3488	6608.3475	0.0013	3	3	1	2	2	0
6620.9276	6620.9217	0.0059	3	3	0	2	2	1
7460.8371	7460.8376	-0.0005	4	3	2	3	2	1
7524.3860	7524.3932	-0.0072	4	3	1	3	2	2
7933.4871	7933.4861	0.0010	8	2	7	7	1	6
7938.7435	7938.7439	-0.0004	10	0	10	9	1	9

Table 14: Observed and calculated rotational transitions (MHz) for singly substituted $^{13}C(4)$.

Observed	Calculated	Obs-Calc	J′	K_a'	K_c'	J″	K_a''	K_c''
3099.1475	3099.1409	0.0066	3	1	3	2	0	2
4712.4294	4712.4338	-0.0044	6	0	6	5	1	5
5120.9784	5120.9746	0.0038	6	1	6	5	0	5
5241.6924	5241.6936	-0.0012	3	2	1	2	1	2
5554.3498	5554.3499	-0.0001	6	2	4	5	2	3
5815.4117	5815.4094	0.0023	7	1	7	6	0	6

6208.8569	6208.8572	-0.0003	5	2	4	4	1	3
6381.5460	6381.5329	0.0131	8	0	8	7	1	7
6402.9353	6402.9370	-0.0017	4	2	2	3	1	3
6587.9218	6587.9226	-0.0008	3	3	1	2	2	0
6600.7917	6600.7926	-0.0009	3	3	0	2	2	1
6815.3444	6815.3510	-0.0066	6	2	5	5	1	4
7508.5115	7508.5061	0.0054	4	3	1	3	2	2
7968.0059	7968.0159	-0.0100	10	0	10	9	1	9

Table 15: Observed and calculated rotational transitions (MHz) for singly substituted $^{13}C(5)$.

Observed	Calculated	Obs-Calc	J′	K_a'	K_c'	J″	K_a''	K_c''
3290.2722	3290.2662	0.0060	4	1	4	3	1	3
4213.2336	4213.2251	0.0085	5	0	5	4	0	4
4457.9170	4457.9269	-0.0099	5	1	5	4	0	4
4736.6559	4736.6573	-0.0014	6	0	6	5	1	5
5249.2040	5249.2068	-0.0028	3	2	1	2	1	2
5482.2387	5482.2379	0.0008	5	4	2	5	3	3
5483.3464	5483.3444	0.0020	4	4	0	4	3	1
5558.1636	5558.1578	0.0058	4	2	3	3	1	2
5587.3164	5587.3165	-0.0001	7	0	7	6	1	6
6586.0030	6586.0082	-0.0052	3	3	1	2	2	0
6599.2315	6599.2323	-0.0008	3	3	0	2	2	1
7394.0564	7394.0539	0.0025	7	2	6	6	1	5
7445.1180	7445.1179	0.0001	4	3	2	3	2	1
7511.9533	7511.9511	0.0022	4	3	1	3	2	2
7740.7269	7740.7277	-0.0008	5	2	3	4	1	4
7946.9211	7946.9244	-0.0033	8	2	7	7	1	6

Table 16: Observed and calculated rotational transitions (MHz) for singly substituted $^{13}C(6)$.

Observed	Calculated	Obs-Calc	J′	K_a'	K_c'	J″	K_a''	K_c''
4226.3629	4226.3767	-0.0138	5	0	5	4	0	4
4751.8269	4751.8264	0.0005	6	0	6	5	1	5
4996.6499	4996.6519	-0.0020	6	0	6	5	0	5
5479.4061	5479.4103	-0.0042	5	4	1	5	3	2
5576.6629	5576.6536	0.0093	4	2	3	3	1	2
5604.8586	5604.8652	-0.0066	7	0	7	6	1	6
5605.0010	5605.0034	-0.0024	6	2	4	5	2	3
6235.0299	6235.0238	0.0061	5	2	4	4	1	3
6443.8029	6443.7946	0.0083	4	2	2	3	1	3
6574.2594	6574.2588	0.0006	8	1	8	7	0	7
6609.5074	6609.5067	0.0007	3	3	1	2	2	0
6622.8434	6622.8532	-0.0098	3	3	0	2	2	1
7315.8428	7315.8341	0.0087	9	1	9	8	0	8
7416.4636	7416.4680	-0.0044	7	2	6	6	1	5
7471.3706	7471.3662	0.0044	4	3	2	3	2	1
7538.8168	7538.8177	-0.0009	4	3	1	3	2	2
7771.3490	7771.3503	-0.0013	5	2	3	4	1	4
7970.5114	7970.5108	0.0006	8	2	7	7	1	6

Table 17: Observed and calculated rotational transitions (MHz) for singly substituted $^{13}C(7)$.

Observed	Calculated	Obs-Calc	J′	K_a'	K_c'	J″	K_a''	K_c''
2392.5160	2392.5176	-0.0016	2	1	2	1	0	1
4466.8370	4466.8306	0.0064	5	1	5	4	0	4
4466.8370	4466.8306	0.0064	5	1	5	4	0	4
4743.6937	4743.6962	-0.0025	6	0	6	5	1	5
5265.5286	5265.5283	0.0003	3	2	1	2	1	2
6231.9290	6231.9309	-0.0019	5	2	4	4	1	3
6419.5135	6419.5159	-0.0024	8	0	8	7	1	7
6438.0193	6438.0192	0.0001	4	2	2	3	1	3

6566.0947	6566.0931	0.0016	8	1	8	7	0	7
6608.9710	6608.9685	0.0025	3	3	1	2	2	0
6622.2164	6622.2152	0.0012	3	3	0	2	2	1
7222.8228	7222.8240	-0.0012	9	0	9	8	1	8
7306.3742	7306.3731	0.0011	9	1	9	8	0	8
7412.1128	7412.1086	0.0042	7	2	6	6	1	5
7536.5374	7536.5426	-0.0052	4	3	1	3	2	2
7762.1468	7762.1449	0.0019	5	2	3	4	1	4
7965.3012	7965.3074	-0.0062	8	2	7	7	1	6

Table 18: Observed and calculated rotational transitions (MHz) for singly substituted $^{13}C(8)$.

Observed	Calculated	Obs-Calc	J′	K_a'	K_c'	J″	K_a''	K_c''
4214.1200	4214.1185	0.0015	2	2	0	1	1	1
5128.6311	5128.6313	-0.0002	6	1	6	5	0	5
5257.3230	5257.3204	0.0026	3	2	1	2	1	2
5568.1030	5568.0992	0.0038	7	0	7	6	1	6
5568.5048	5568.5040	0.0008	4	2	3	3	1	2
5823.5918	5823.5820	0.0098	7	1	7	6	0	6
6389.4276	6389.4176	0.0100	8	0	8	7	1	7
6420.9151	6420.9182	-0.0031	4	2	2	3	1	3
6541.1117	6541.1111	0.0006	8	1	8	7	0	7
6622.8000	6622.7932	0.0068	3	3	0	2	2	1
7400.4879	7400.4906	-0.0027	7	2	6	6	1	5
7466.6573	7466.6540	0.0033	4	3	2	3	2	1
7531.9022	7531.9116	-0.0094	4	3	1	3	2	2
7951.1039	7951.1059	-0.0020	8	2	7	7	1	6
7977.9296	7977.9438	-0.0142	10	0	10	9	1	9

Table 19: Observed and calculated rotational transitions (MHz) for singly substituted $^{13}C(9)$.

Observed	Calculated	Obs-Calc	J′	K_a′	K_c′	J″	K_a″	K_c″
4441.3486	4441.3526	-0.0040	5	1	5	4	0	4
4704.2804	4704.2787	0.0017	6	0	6	5	1	5
4844.9969	4844.9979	-0.0010	3	2	2	2	1	1
5114.1066	5114.1057	0.0009	6	1	6	5	0	5
5243.7193	5243.7209	-0.0016	3	2	1	2	1	2
5509.7784	5509.7696	0.0088	6	4	3	6	3	4
5807.0075	5807.0060	0.0015	7	1	7	6	0	6
6207.3777	6207.3763	0.0014	5	2	4	4	1	3
6371.0747	6371.0731	0.0016	8	0	8	7	1	7
6522.4347	6522.4310	0.0037	8	1	8	7	0	7
6593.1395	6593.1368	0.0027	3	3	1	2	2	0
6606.0155	6606.0166	-0.0011	3	3	0	2	2	1
6812.2637	6812.2698	-0.0061	6	2	5	5	1	4
7380.2372	7380.2414	-0.0042	7	2	6	6	1	5
7447.4780	7447.4790	-0.0010	4	3	2	3	2	1
7512.5701	7512.5762	-0.0061	4	3	1	3	2	2
7955.0482	7955.0440	0.0042	10	0	10	9	1	9

Table 20: Observed and calculated rotational transitions (MHz) for singly substituted $^{13}C(10)$.

Observed	Calculated	Obs-Calc	J′	K_a′	K_c′	J″	K_a″	K_c″
3088.9764	3088.9725	0.0039	3	1	3	2	0	2
3768.5374	3768.5351	0.0023	4	1	4	3	0	3
4049.2431	4049.2384	0.0047	2	2	1	1	1	0
4176.9483	4176.9434	0.0049	2	2	0	1	1	1
4435.1765	4435.1746	0.0019	5	1	5	4	0	4
4723.3499	4723.3545	-0.0046	6	0	6	5	1	5
5110.4916	5110.4928	-0.0012	6	1	6	5	0	5
5525.8983	5525.8935	0.0048	4	2	3	3	1	2
5569.0821	5569.0812	0.0009	7	0	7	6	1	6

6178.6995	6178.6985	0.0010	5	2	4	4	1	3
6395.9360	6395.9309	0.0051	4	2	2	3	1	3
6525.6930	6525.6809	0.0121	8	1	8	7	0	7
6545.1600	6545.1595	0.0005	3	3	1	2	2	0
6558.6942	6558.7053	-0.0111	3	3	0	2	2	1
6782.4525	6782.4541	-0.0016	6	2	5	5	1	4
7183.9455	7183.9484	-0.0029	9	0	9	8	1	8
7401.2413	7401.2485	-0.0072	4	3	2	3	2	1
7469.7073	7469.7032	0.0041	4	3	1	3	2	2
7968.9183	7968.9266	-0.0083	10	0	10	9	1	9

Table 21: Observed and calculated rotational transitions (MHz) for singly substituted $^{13}C(11)$.

Observed	Calculated	Obs-Calc	J′	K_a'	K_c'	J″	K_a''	K_c''
3782.1532	3782.1599	-0.0067	4	1	4	3	0	3
4451.7323	4451.7340	-0.0017	5	1	5	4	0	4
4744.8039	4744.8177	-0.0138	6	0	6	5	1	5
5240.8537	5240.8537	0.0000	3	2	1	2	1	2
5542.5551	5542.5509	0.0042	4	2	3	3	1	2
5593.5979	5593.5991	-0.0012	7	0	7	6	1	6
6197.9597	6197.9496	0.0101	5	2	4	4	1	3
6418.1911	6418.2005	-0.0094	4	2	2	3	1	3
6561.9062	6561.9127	-0.0065	3	3	1	2	2	0
6575.5977	6575.5972	0.0005	3	3	0	2	2	1
7373.7624	7373.7620	0.0004	7	2	6	6	1	5
7421.6145	7421.6136	0.0009	4	3	2	3	2	1
7490.7683	7490.7681	0.0002	4	3	1	3	2	2
7749.7728	7749.7732	-0.0004	5	2	3	4	1	4
7749.7798	7749.7732	0.0066	5	2	3	4	1	4
7926.1716	7926.1723	-0.0007	8	2	7	7	1	6

Table 22: Observed and calculated rotational transitions (MHz) for singly substituted $^{13}C(12)$.

Observed	Calculated	Obs-Calc	J′	K_a'	K_c'	J″	K_a''	K_c''
2934.0851	2934.0861	-0.0010	4	0	4	3	1	3
4217.5951	4217.6013	-0.0062	2	2	0	1	1	1
5268.8767	5268.8759	0.0008	3	2	1	2	1	2
6119.3521	6119.3534	-0.0013	7	2	6	6	2	5
6425.8926	6425.8930	-0.0004	8	0	8	7	1	7
6442.8193	6442.8130	0.0063	4	2	2	3	1	3
6612.0404	6612.0366	0.0038	3	3	1	2	2	0
6625.3234	6625.3211	0.0023	3	3	0	2	2	1
6844.9232	6844.9217	0.0015	6	2	5	5	1	4
7229.8635	7229.8730	-0.0095	9	0	9	8	1	8
7313.1514	7313.1411	0.0103	9	1	9	8	0	8
7417.0830	7417.0838	-0.0008	7	2	6	6	1	5
7473.4892	7473.4936	-0.0044	4	3	2	3	2	1
7540.6291	7540.6326	-0.0035	4	3	1	3	2	2
7768.6710	7768.6714	-0.0004	5	2	3	4	1	4
7970.8638	7970.8632	0.0006	8	2	7	7	1	6

Table 23: Observed and calculated rotational transitions (MHz) for singly substituted $^{13}C(13)$.

Observed	Calculated	Obs-Calc	J′	K_a'	K_c'	J″	K_a''	K_c''
3098.0361	3098.0344	0.0017	3	1	3	2	0	2
4449.7078	4449.7070	0.0008	5	1	5	4	0	4
4744.1118	4744.1144	-0.0026	6	0	6	5	1	5
5128.1026	5128.0924	0.0102	6	1	6	5	0	5
5237.1601	5237.1602	-0.0001	3	2	1	2	1	2
5538.4457	5538.4485	-0.0028	4	2	3	3	1	2
5592.4635	5592.4725	-0.0090	7	0	7	6	1	6
5827.6551	5827.6492	0.0059	7	1	7	6	0	6
6193.6302	6193.6179	0.0123	5	2	4	4	1	3
6412.4085	6412.4111	-0.0026	8	0	8	7	1	7

6414.5469	6414.5463	0.0006	4	2	2	3	1	3
6569.5776	6569.5813	-0.0037	3	3	0	2	2	1
6799.5463	6799.5462	0.0001	6	2	5	5	1	4
7369.0471	7369.0558	-0.0087	7	2	6	6	1	5
7415.3365	7415.3366	-0.0001	4	3	2	3	2	1
7484.6210	7484.6235	-0.0025	4	3	1	3	2	2
7746.2769	7746.2734	0.0035	5	2	3	4	1	4

8.3 BPCO-1w(I)-^{16}O

Table 24: Observed and calculated rotational transitions (MHz) for BPCO-1w(I)-^{16}O.

Observed	Calculated	Obs-Calc	J′	K_a′	K_c′	J″	K_a″	K_c″
2328.2674	2328.2710	-0.0036	3	1	3	2	0	2
2371.3450	2371.3461	-0.0011	4	1	4	3	1	3
2475.1764	2475.1900	-0.0136	4	0	4	3	0	3
2538.9081	2538.9129	-0.0048	4	2	3	3	2	2
2560.4588	2560.4510	0.0078	4	3	1	3	3	0
2608.2951	2608.2873	0.0078	4	2	2	3	2	1
2688.5686	2688.5691	-0.0005	4	1	3	3	1	2
2705.7546	2705.7524	0.0022	5	0	5	4	1	4
2819.8897	2819.8889	0.0008	4	1	4	3	0	3
2953.1329	2953.1327	0.0002	5	1	5	4	1	4
3050.4472	3050.4513	-0.0041	5	0	5	4	0	4
3164.5691	3164.5694	-0.0003	5	2	4	4	2	3
3201.6596	3201.6588	0.0008	5	3	3	4	3	2
3202.4103	3202.4070	0.0033	2	2	1	1	1	0
3210.2483	3210.2477	0.0006	5	3	2	4	3	1
3289.6098	3289.6096	0.0002	2	2	0	1	1	1
3294.6904	3294.6885	0.0019	5	2	3	4	2	2
3297.8210	3297.8316	-0.0106	5	1	5	4	0	4
3344.1708	3344.1740	-0.0032	5	1	4	4	1	3
3362.4101	3362.4120	-0.0019	6	0	6	5	1	5
3529.4312	3529.4305	0.0007	6	1	6	5	1	5

3609.7898	3609.7924	-0.0026	6	0	6	5	0	5
3758.6210	3758.6259	-0.0049	3	2	2	2	1	1
3776.8108	3776.8109	-0.0001	6	1	6	5	0	5
3784.3162	3784.3157	0.0005	6	2	5	5	2	4
3846.2729	3846.2708	0.0021	6	3	4	5	3	3
3868.6847	3868.6837	0.0010	6	3	3	5	3	2
3986.5640	3986.5648	-0.0008	6	1	5	5	1	4
3990.6891	3990.6897	-0.0006	6	2	4	5	2	3
3993.3924	3993.3877	0.0047	7	0	7	6	1	6
4034.3947	4034.3930	0.0017	3	2	1	2	1	2
4100.6281	4100.6317	-0.0036	7	1	7	6	1	6
4160.4076	4160.4062	0.0014	7	0	7	6	0	6
4267.6489	4267.6502	-0.0013	7	1	7	6	0	6
4273.9797	4273.9833	-0.0036	4	2	3	3	1	2
4397.2116	4397.2121	-0.0005	7	2	6	6	2	5
4490.5003	4490.5013	-0.0010	7	3	5	6	3	4
4490.6707	4490.6680	0.0027	7	4	3	6	4	2
4539.0927	4539.0941	-0.0014	7	3	4	6	3	3
4601.2543	4601.2587	-0.0044	8	0	8	7	1	7
4611.4744	4611.4721	0.0023	7	1	6	6	1	5
4667.4881	4667.4859	0.0022	8	1	8	7	1	7
4687.5010	4687.4959	0.0051	7	2	5	6	2	4
4708.4962	4708.5027	-0.0065	8	0	8	7	0	7
4749.9791	4749.9837	-0.0046	5	2	4	4	1	3
4774.7298	4774.7299	-0.0001	8	1	8	7	0	7
4858.4719	4858.4885	-0.0166	4	2	2	3	1	3
5002.5654	5002.5627	0.0027	8	2	7	7	2	6
5002.5655	5002.5627	0.0028	8	2	7	7	2	6
5124.8284	5124.8170	0.0114	8	5	4	7	5	3
5125.0019	5125.0003	0.0016	8	5	3	7	5	2
5132.7034	5132.7013	0.0021	8	3	6	7	3	5
5137.7284	5137.7362	-0.0078	8	4	5	7	4	4
5144.0166	5144.0078	0.0088	8	4	4	7	4	3
5188.9713	5188.9711	0.0002	3	3	1	2	2	0
5190.1292	5190.1255	0.0037	6	2	5	5	1	4
5191.2044	5191.2060	-0.0016	9	0	9	8	1	8

5196.6565	5196.6630	-0.0065	3	3	0	2	2	1
5215.1206	5215.1234	-0.0028	8	1	7	7	1	6
5224.2782	5224.2827	-0.0045	8	3	5	7	3	4
5230.9027	5230.9045	-0.0018	9	1	9	8	1	8
5257.4305	5257.4332	-0.0027	9	0	9	8	0	8
5297.1371	5297.1317	0.0054	9	1	9	8	0	8
5376.9346	5376.9317	0.0029	8	2	6	7	2	5
5600.0108	5600.0085	0.0023	9	2	8	8	2	7
5600.7728	5600.7728	0.0000	7	2	6	6	1	5
5768.5311	5768.5269	0.0042	10	0	10	9	1	9
5771.0998	5771.0905	0.0093	9	3	7	8	3	6
5776.0193	5776.0215	-0.0022	10	1	9	9	2	8
5781.8371	5781.8309	0.0062	5	2	3	4	1	4
5789.1646	5789.1655	-0.0009	9	4	6	8	4	5
5791.7784	5791.7849	-0.0065	10	1	10	9	1	9
5796.0355	5796.0324	0.0031	9	1	8	8	1	7
5803.8459	5803.8523	-0.0064	9	4	5	8	4	4
5808.2246	5808.2254	-0.0008	10	0	10	9	0	9
5809.7912	5809.7894	0.0018	4	3	2	3	2	1
5831.4812	5831.4834	-0.0022	10	1	10	9	0	9
5848.6711	5848.6750	-0.0039	4	3	1	3	2	2
5924.6920	5924.6965	-0.0045	9	3	6	8	3	5
5991.8633	5991.8633	-0.0000	8	2	7	7	1	6
6053.1485	6053.1568	-0.0083	9	2	7	8	2	6
6350.9029	6350.8980	0.0049	11	1	11	10	1	10
6356.7411	6356.7377	0.0034	10	1	9	9	1	8
6360.7738	6360.7726	0.0012	11	0	11	10	0	10
6374.1570	6374.1561	0.0009	11	1	11	10	0	10
6376.7531	6376.7485	0.0046	9	2	8	8	1	7
6403.1627	6403.1609	0.0018	5	3	3	4	2	2
6403.9703	6403.9660	0.0043	10	3	8	9	3	7
6441.8498	6441.8507	-0.0009	10	4	7	9	4	6
6472.5460	6472.5562	-0.0102	10	4	6	9	4	5
6520.0124	6520.0098	0.0026	5	3	2	4	2	3
6636.6266	6636.6284	-0.0018	10	3	7	9	3	6
6712.0269	6712.0298	-0.0029	10	2	8	9	2	7

6770.3151	6770.3106	0.0045	10	2	9	9	1	8
6771.7838	6771.7811	0.0027	11	2	10	10	2	9
6819.3948	6819.3879	0.0069	6	2	4	5	1	5
6903.6507	6903.6475	0.0032	11	1	10	10	1	9
6908.8330	6908.8414	-0.0084	12	1	12	11	1	11
6954.7466	6954.7432	0.0034	6	3	4	5	2	3
7029.8795	7029.8674	0.0121	11	3	9	10	3	8
7094.5902	7094.5888	0.0014	11	4	8	10	4	7
7142.2824	7142.2875	-0.0051	4	4	1	3	3	0
7142.7282	7142.7232	0.0050	4	4	0	3	3	1
7152.9480	7152.9513	-0.0033	11	4	7	10	4	6
7224.1260	7224.1241	0.0019	6	3	3	5	2	4
7347.3912	7347.3872	0.0040	12	2	11	11	2	10
7350.0416	7350.0412	0.0004	11	2	9	10	2	8
7352.2904	7352.2848	0.0056	11	3	8	10	3	7
7444.3953	7444.3892	0.0061	12	1	11	11	1	10
7454.5576	7454.5548	0.0028	7	3	5	6	2	4
7461.7874	7461.7891	-0.0017	13	0	13	12	1	12
7466.0398	7466.0435	-0.0037	13	1	13	12	1	12
7469.3858	7469.3799	0.0059	13	0	13	12	0	12
7647.6806	7647.6900	-0.0094	12	3	10	11	3	9
7742.1846	7742.1948	-0.0102	12	5	7	11	5	6
7745.8244	7745.8276	-0.0032	12	4	9	11	4	8
7778.7174	7778.7196	-0.0022	5	4	2	4	3	1
7781.7960	7781.7952	0.0008	5	4	1	4	3	2
7847.6940	7847.7110	-0.0170	12	4	8	11	4	7
7899.7580	7899.7602	-0.0022	8	3	6	7	2	5
7917.4812	7917.4685	0.0127	13	2	12	12	2	11
7964.1233	7964.1293	-0.0060	12	2	10	11	2	9
7978.8993	7978.9025	-0.0032	7	3	4	6	2	5
7984.8102	7984.7973	0.0129	13	1	12	12	1	11

8.4 BPCO-1w(I)-^{18}O

Table 25: Observed and calculated rotational transitions (MHz) for BPCO-1w(I)-^{18}O.

Observed	Calculated	Obs-Calc	J′	K_a′	K_c′	J″	K_a″	K_c″
2282.1355	2282.1345	0.0010	3	1	3	2	0	2
2304.2170	2304.2124	0.0046	4	1	4	3	1	3
2405.4984	2405.4968	0.0016	4	0	4	3	0	3
2607.0190	2607.0214	-0.0024	4	1	3	3	1	2
2870.1060	2870.1067	-0.0007	5	1	5	4	1	4
2966.4991	2966.5028	-0.0037	5	0	5	4	0	4
3071.4467	3071.4447	0.0020	5	2	4	4	2	3
3190.9690	3190.9675	0.0015	5	2	3	4	2	2
3243.8437	3243.8417	0.0020	5	1	4	4	1	3
3253.0744	3253.0758	-0.0014	6	0	6	5	1	5
3430.8911	3430.8787	0.0124	6	1	6	5	1	5
3511.9999	3512.0029	-0.0030	6	0	6	5	0	5
3673.7353	3673.7315	0.0038	6	2	5	5	2	4
3706.8730	3706.8721	0.0009	3	2	2	2	1	1
3730.5498	3730.5466	0.0032	6	3	4	5	3	3
3864.5285	3864.5290	-0.0005	6	2	4	5	2	3
3868.7842	3868.7832	0.0010	6	1	5	5	1	4
3870.6316	3870.6324	-0.0008	7	0	7	6	1	6
3968.3938	3968.3911	0.0027	3	2	1	2	1	2
3986.8293	3986.8325	-0.0032	7	1	7	6	1	6
4048.4331	4048.4353	-0.0022	7	0	7	6	0	6
4269.7454	4269.7483	-0.0029	7	2	6	6	2	5
4355.5563	4355.5553	0.0010	7	3	5	6	3	4
4477.9790	4477.9772	0.0018	7	1	6	6	1	5
4538.6143	4538.6128	0.0015	8	1	8	7	1	7
4540.0027	4539.9968	0.0059	7	2	5	6	2	4
4581.7750	4581.7727	0.0023	8	0	8	7	0	7
4673.3265	4673.3369	-0.0104	5	2	4	4	1	3
4858.8263	4858.8238	0.0025	8	2	7	7	2	6
5059.4976	5059.4937	0.0039	8	3	5	7	3	4
5067.8286	5067.8273	0.0013	8	1	7	7	1	6

5087.0361	5087.0354	0.0007	9	1	9	8	1	8
5115.5200	5115.5179	0.0021	9	0	9	8	0	8
5209.6625	5209.6665	-0.0040	8	2	6	7	2	5
5440.5980	5440.5737	0.0243	9	2	8	8	2	7
5599.0496	5599.0427	0.0069	9	5	4	8	5	3
5599.0496	5599.0573	-0.0077	9	3	7	8	3	6
5613.6616	5613.6631	-0.0015	9	4	6	8	4	5
5625.9100	5625.9021	0.0079	9	4	5	8	4	4
5632.9240	5632.9293	-0.0053	10	1	10	9	1	9
5636.4882	5636.4819	0.0063	9	1	8	8	1	7
5650.9293	5650.9248	0.0045	10	0	10	9	0	9
5735.3046	5735.3035	0.0011	9	3	6	8	3	5
5867.8570	5867.8592	-0.0022	9	2	7	8	2	6
6014.9684	6014.9645	0.0039	10	2	9	9	2	8
6177.0214	6177.0260	-0.0046	11	1	11	10	1	10
6185.4708	6185.4742	-0.0034	10	1	9	9	1	8
6188.0465	6188.0381	0.0084	11	0	11	10	0	10
6257.7811	6257.7848	-0.0037	9	2	8	8	1	7
6422.9213	6422.9197	0.0016	10	3	7	9	3	6
6510.5970	6510.5956	0.0014	10	2	8	9	2	7
6582.3575	6582.3356	0.0219	11	2	10	10	2	9
6719.9054	6719.9082	-0.0028	12	1	12	11	1	11
6720.0339	6720.0283	0.0056	11	1	10	10	1	9
6726.4882	6726.4865	0.0017	12	0	12	11	0	11
6823.4568	6823.4547	0.0021	11	3	9	10	3	8
6879.5119	6879.4984	0.0135	11	4	8	10	4	7
7115.8879	7115.9067	-0.0188	11	3	8	10	3	7
7134.6074	7134.6077	-0.0003	11	2	9	10	2	8
7143.3741	7143.3617	0.0124	12	2	11	11	2	10
7247.1351	7247.1238	0.0113	12	1	11	11	1	10
7262.0157	7262.0041	0.0116	13	1	13	12	1	12
7425.2550	7425.2482	0.0068	12	3	10	11	3	9
7597.8464	7597.8696	-0.0232	12	4	8	11	4	7
7736.9513	7736.9631	-0.0118	12	2	10	11	2	9
7772.6777	7772.6945	-0.0168	13	1	12	12	1	11
7782.6228	7782.6212	0.0016	8	3	6	7	2	5

7803.5962	7803.6093	-0.0131	14	1	14	13	1	13
7805.8037	7805.8373	-0.0336	14	0	14	13	0	13

8.5 BPCO-1w(II)-^{16}O

Table 26: Observed and calculated rotational transitions (MHz) for BPCO-1w(II)-^{16}O.

Observed	Calculated	Obs-Calc	J′	K_a′	K_c′	J″	K_a″	K_c″
2010.9353	2010.9369	-0.0016	3	0	3	2	1	2
2066.1256	2066.1252	0.0004	3	1	3	2	0	2
2178.8546	2178.8494	0.0052	2	2	1	1	1	0
2189.0570	2189.0558	0.0012	3	1	2	2	2	1
2499.2390	2499.2339	0.0051	2	2	0	1	1	1
2625.4846	2625.4812	0.0034	4	0	4	3	1	3
2637.9286	2637.9359	-0.0073	4	1	4	3	0	3
2771.9419	2771.9399	0.0020	3	2	2	2	1	1
2793.2837	2793.2704	0.0133	7	3	5	7	2	6
3013.5616	3013.5649	-0.0033	4	1	3	3	2	2
3223.2879	3223.2909	-0.0030	5	0	5	4	1	4
3225.6398	3225.6421	-0.0023	5	1	5	4	0	4
3277.7172	3277.7144	0.0028	4	2	3	3	1	2
3477.7559	3477.7446	0.0113	3	3	1	2	2	0
3648.6980	3648.6902	0.0078	3	3	0	2	2	1
3704.7471	3704.7437	0.0034	5	1	4	4	2	3
3789.2561	3789.2418	0.0143	5	2	4	4	1	3
3817.2072	3817.2091	-0.0019	6	0	6	5	1	5
3817.6115	3817.6117	-0.0002	6	1	6	5	0	5
3826.8146	3826.8246	-0.0100	3	2	1	2	1	2
3865.5143	3865.5172	-0.0029	5	2	3	4	3	2
4092.1090	4092.1094	-0.0004	4	3	2	3	2	1
4327.4246	4327.4208	0.0038	6	1	5	5	2	4
4348.1907	4348.1861	0.0046	6	2	5	5	1	4
4410.3872	4410.3935	-0.0063	7	0	7	6	1	6
4410.4579	4410.4583	-0.0004	7	1	7	6	0	6

4580.1155	4580.1135	0.0020	5	3	3	4	2	2
4712.8205	4712.8220	-0.0015	6	2	4	5	3	3
4775.8440	4775.8303	0.0137	4	4	1	3	3	0
4819.0730	4819.0728	0.0002	4	3	1	3	2	2
4848.0335	4848.0322	0.0013	4	4	0	3	3	1
4931.6874	4931.6782	0.0092	7	2	6	6	1	5
5003.4616	5003.4745	-0.0129	8	1	8	7	0	7
5003.4616	5003.4645	-0.0029	8	0	8	7	1	7
5409.3137	5409.3052	0.0085	7	2	5	6	3	4
5450.4692	5450.4607	0.0085	5	4	2	4	3	1
5522.3102	5522.3111	-0.0009	8	2	7	7	1	6
5596.5168	5596.5244	-0.0076	9	0	9	8	1	8
5596.5168	5596.5259	-0.0091	9	1	9	8	0	8
5870.4742	5870.4808	-0.0066	5	4	1	4	3	2
5907.9953	5907.9971	-0.0018	4	3	2	3	0	3
5958.0424	5958.0459	-0.0035	6	4	3	5	3	2
6033.4005	6033.3958	0.0047	8	2	6	7	3	5
6053.7632	6053.7568	0.0064	5	5	1	4	4	0
6058.5811	6058.5783	0.0028	8	3	6	7	2	5
6079.6470	6079.6405	0.0065	5	5	0	4	4	1
6288.7375	6288.7456	-0.0081	5	3	2	4	2	3
6428.4377	6428.4220	0.0157	8	3	5	7	4	4
6633.3167	6633.3078	0.0089	9	2	7	8	3	6
6638.9616	6638.9545	0.0071	9	3	7	8	2	6
6707.4324	6707.4182	0.0142	10	1	9	9	2	8
6746.7885	6746.7938	-0.0053	8	4	5	7	3	4
6782.6217	6782.6420	-0.0203	11	1	11	10	0	10
6801.7291	6801.7350	-0.0059	6	5	2	5	4	1
7003.1648	7003.1803	-0.0155	6	5	1	5	4	2
7120.7459	7120.7340	0.0119	9	3	6	8	4	5
7175.2280	7175.2523	-0.0243	6	4	2	5	3	3
7221.9313	7221.9328	-0.0015	9	4	6	8	3	5
7317.6497	7317.6485	0.0012	6	6	1	5	5	0
7326.0506	7326.0464	0.0042	6	6	0	5	5	1
7366.7265	7366.7236	0.0029	5	3	3	4	0	4
7375.6707	7375.6667	0.0040	12	1	12	11	0	11

7377.4485	7377.4624	-0.0139	7	5	3	6	4	2
7742.5760	7742.5641	0.0119	10	3	7	9	4	6
7781.1721	7781.1872	-0.0151	8	5	4	7	4	3

8.6 BPCO-1w(II)-^{18}O

Table 27: Observed and calculated rotational transitions (MHz) for BPCO-1w(II)-^{18}O.

Observed	Calculated	Obs-Calc	J′	K_a′	K_c′	J″	K_a″	K_c″
2570.1250	2570.1377	-0.0127	4	0	4	3	1	3
2576.3338	2576.3350	-0.0012	4	1	4	3	0	3
2666.7810	2666.7629	0.0181	3	2	2	2	1	1
2998.5248	2998.5283	-0.0035	4	1	3	3	2	2
3153.2543	3153.2589	-0.0046	5	1	5	4	0	4
3165.3270	3165.3152	0.0118	4	2	3	3	1	2
3322.7922	3322.7755	0.0167	3	3	1	2	2	0
3529.7581	3529.7401	0.0180	3	3	0	2	2	1
3642.3678	3642.3677	0.0001	5	1	4	4	2	3
3685.2470	3685.2497	-0.0027	5	2	4	4	1	3
3685.2470	3685.2359	0.0111	11	5	7	11	4	8
3916.7426	3916.7209	0.0217	4	3	2	3	2	1
3924.1421	3924.1492	-0.0071	5	2	3	4	3	2
4237.5618	4237.5456	0.0162	6	1	5	5	2	4
4245.9673	4245.9643	0.0030	6	2	5	5	1	4
4312.1722	4312.1922	-0.0200	7	1	7	6	0	6
4389.6519	4389.6390	0.0129	5	3	3	4	2	2
4666.2875	4666.2818	0.0057	4	4	0	3	3	1
4756.4326	4756.4228	0.0098	4	3	1	3	2	2
4891.9091	4891.9155	-0.0064	8	0	8	7	1	7
4891.9091	4891.9175	-0.0084	8	1	8	7	0	7
5203.8870	5203.8810	0.0060	5	4	2	4	3	1
5314.7866	5314.7882	-0.0016	7	2	5	6	3	4
5355.6601	5355.6584	0.0017	7	3	5	6	2	4
5471.6473	5471.6537	-0.0064	9	1	9	8	0	8

5638.8175	5638.8220	-0.0045	7	3	4	6	4	3
5679.3319	5679.3188	0.0131	6	4	3	5	3	2
5755.0838	5755.0899	-0.0061	5	4	1	4	3	2
5790.7627	5790.7856	-0.0229	5	5	1	4	4	0
5833.8984	5833.9169	-0.0185	5	5	0	4	4	1
5907.2998	5907.2892	0.0106	8	2	6	7	3	5
5915.6459	5915.6365	0.0094	8	3	6	7	2	5
5979.5385	5979.5421	-0.0036	9	2	8	8	1	7
5979.5385	5979.5111	0.0274	9	1	8	8	2	7
6051.3868	6051.4027	-0.0159	10	0	10	9	1	9
6051.3868	6051.3903	-0.0035	10	1	10	9	0	9
6072.8215	6072.8070	0.0145	7	4	4	6	3	3
6488.7502	6488.7389	0.0113	9	2	7	8	3	6
6490.2383	6490.2351	0.0032	9	3	7	8	2	6
6499.1553	6499.1740	-0.0187	6	5	2	5	4	1
6506.8148	6506.8174	-0.0026	8	4	5	7	3	4
6810.2974	6810.3260	-0.0286	6	5	1	5	4	2
7015.3557	7015.3721	-0.0164	7	5	3	6	4	2
7578.5363	7578.5275	0.0088	10	3	7	9	4	6

8.7 BPCO-2w(II)-^{16}O-^{16}O

Table 28: Observed and calculated rotational transitions (MHz) for BPCO-2w(II)-^{16}O-^{16}O.

Observed	Calculated	Obs-Calc	J′	K_a′	K_c′	J″	K_a″	K_c″
2206.0592	2206.0574	0.0018	3	1	2	2	1	1
2412.4580	2412.4542	0.0038	3	2	1	2	2	0
2712.3658	2712.3662	-0.0004	4	1	3	3	1	2
3129.3439	3129.3432	0.0007	4	2	2	3	2	1
3198.0168	3198.0250	-0.0082	5	1	4	4	2	3
3199.6650	3199.6642	0.0008	5	2	4	4	2	3
3209.3924	3209.3915	0.0009	5	1	4	4	1	3
3211.0301	3211.0306	-0.0005	5	2	4	4	1	3
3212.1455	3212.1485	-0.0030	4	3	1	3	3	0

3306.1321	3306.1290	0.0031	6	1	6	5	1	5
3561.2166	3561.2167	-0.0001	5	3	3	4	3	2
3677.5367	3677.5343	0.0024	5	2	3	4	2	2
3969.2358	3969.2355	0.0003	5	4	1	4	4	0
4015.6340	4015.6324	0.0016	5	3	2	4	3	1
4113.7186	4113.7212	-0.0026	6	2	4	5	3	3
4121.6690	4121.6694	-0.0004	6	3	4	5	3	3
4156.7845	4156.7868	-0.0023	6	2	4	5	2	3
4164.7375	4164.7350	0.0025	6	3	4	5	2	3
4164.8000	4164.7994	0.0006	4	3	1	3	1	2
4339.2239	4339.2238	0.0001	8	1	8	7	1	7
4339.2239	4339.2239	-0.0000	8	0	8	7	0	7
4435.6544	4435.6536	0.0008	6	4	3	5	4	2
4558.4030	4558.4002	0.0028	6	5	2	5	5	1
4594.3916	4594.3954	-0.0038	5	4	1	4	3	1
4641.1266	4641.1258	0.0008	6	3	3	5	3	2
4642.5456	4642.5457	-0.0001	5	3	3	4	2	3
4649.3178	4649.3136	0.0042	7	3	5	6	3	4
4656.0735	4656.0761	-0.0026	7	2	5	6	2	4
5033.5130	5033.5139	-0.0009	7	4	4	6	4	3
5269.3170	5269.3165	0.0005	9	2	8	8	2	7
5269.3170	5269.3186	-0.0016	9	1	8	8	1	7
5285.7212	5285.7270	-0.0058	7	5	3	6	5	2
5577.3088	5577.3059	0.0029	8	4	5	7	4	4
5578.9873	5578.9860	0.0013	7	4	3	6	4	2
5929.5797	5929.5776	0.0021	8	5	4	7	5	3
6293.0305	6293.0301	0.0004	6	4	2	5	2	3
6500.2076	6500.2086	-0.0010	9	5	5	8	5	4

8.8 BPCO-2w(II)-^{18}O(1)-^{16}O(2)

Table 29: Observed and calculated rotational transitions (MHz) for BPCO-2w(II)-^{18}O(1)-^{16}O(2).

Observed	Calculated	Obs-Calc	J′	K_a′	K_c′	J″	K_a″	K_c″
4107.1705	4107.1690	0.0015	6	2	4	5	2	3
4182.5860	4182.5870	-0.0010	7	2	6	6	2	5
4182.8773	4182.8697	0.0076	7	1	6	6	1	5
4356.7392	4356.7446	-0.0054	6	4	3	5	4	2
4577.7260	4577.7231	0.0029	6	3	3	5	3	2
4587.3182	4587.3158	0.0024	7	3	5	6	3	4
4596.8462	4596.8433	0.0029	7	2	5	6	2	4
4692.9750	4692.9768	-0.0018	8	2	7	7	2	6
4751.1455	4751.1434	0.0021	6	4	2	5	4	1
4797.2443	4797.2430	0.0013	9	0	9	8	0	8
4797.2443	4797.2429	0.0014	9	1	9	8	1	8
4956.3625	4956.3600	0.0025	7	4	4	6	4	3
5100.0170	5100.0221	-0.0051	8	3	6	7	3	5
5101.6236	5101.6332	-0.0096	8	2	6	7	2	5

8.9 BPCO-2w(II)-^{16}O(1)-^{18}O(2)

Table 30: Observed and calculated rotational transitions (MHz) for BPCO-2w(II)-^{16}O(1)-^{18}O(2).

Observed	Calculated	Obs-Calc	J′	K_a′	K_c′	J″	K_a″	K_c″
3611.5000	3611.4945	0.0055	5	2	3	4	2	2
3653.4093	3653.4146	-0.0053	6	2	5	5	2	4
3753.7672	3753.7628	0.0044	7	0	7	6	0	6
3753.7672	3753.7615	0.0057	7	1	7	6	1	6
4049.9640	4049.9628	0.0012	6	3	4	5	3	3
4260.9362	4260.9361	0.0001	8	0	8	7	0	7
4260.9362	4260.9360	0.0002	8	1	8	7	1	7
4559.4509	4559.4518	-0.0009	6	3	3	5	3	2
4567.3173	4567.3243	-0.0070	7	3	5	6	3	4

4573.3389	4573.3373	0.0016	7	2	5	6	2	4
4768.1074	4768.1096	-0.0022	9	0	9	8	0	8
4768.1074	4768.1096	-0.0022	9	1	9	8	1	8
4782.2606	4782.2596	0.0010	6	4	2	5	4	1