Electronic Supplementary Information.

"Next Generation Techniques in the High Resolution Spectroscopy of Biologically Relevant Molecules", by J. L. Neill, K. O. Douglass, B. H. Pate, and D. W. Pratt

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Table S1. Observed transitions of the singly hydrated complex of conformer D of *p*MPEA.

J'	Ka'	Kc'	F'	J''	Ka''	Kc''	F''	Frequency (MHz)	Obs-calc (kHz)
8	3	5	8	8	2	6	8	6481.482	-21.1
8	3	5	9,7[a]	8	2	6	9,7	6481.690	-13.0
5	3	2	5	5	2	3	5	6640.440	-7.4
5	3	2	6,4	5	2	3	6,4	6640.560	-17.5
5	3	3	[b]	5	2	4		6689.342	-1.5
5	3	2		5	2	4		6690.046	-3.5
6	3	4		6	2	5		6702.920	-8.7
6	3	3		6	2	5		6705.038	-5.6
7	3	5		7	2	6		6724.312	-29.3
7	3	4		7	2	6		6729.586	-29.6
8	3	6		8	2	7		6755.804	-14.1
8	3	5		8	2	7		6767.364	-15.0
9	3	7		9	2	8		6799.666	-26.2
9	3	6		9	2	8		6822.656	-36.8
10	3	8	11,9	10	2	9	11,9	6858.284	-2.9
10	3	8	10	10	2	9	10	6858.384	-5.4
10	3	7	11,9	10	2	9	11,9	6900.682	4.5
10	3	7	10	10	2	9	10	6900.820	-1.5
11	3	9	12,10	11	2	10	12,10	6933.972	-0.1
11	3	9	11	11	2	10	11	6934.094	-1.3
11	3	8	12,10	11	2	10	12,10	7007.436	5.5
11	3	8	11	11	2	10	11	7007.614	0.6
8	1	8	8	7	0	7	7	7024.122	2.0
8	1	8	9,7	7	0	7	8,6	7024.394	-28.7
12	3	10	13,11	12	2	11	13,11	7028.922	9.4
12	3	10	12	12	2	11	12	7029.068	11.8
4	2	3	4	3	1	2	3	7096.728	-0.6
4	2	3	5	3	1	2	4	7097.156	-2.5
4	2	3	3	3	1	2	2	7097.316	4.4
4	2	2	4	3	1	2	3	7118.100	-5.1
4	2	2	5	3	1	2	4	7118.464	-0.9
4	2	2	3	3	1	2	2	7118.602	2.1
13	3	11	14,12	13	2	12	14,12	7145.126	5.9
13	3	11	13	13	2	12	13	7145.294	10.5
12	3	9	13,11	12	2	11	13,11	7149.778	18.6
14	3	12	15,13	14	2	13	15,13	7284.374	1.9
14	3	12	14	14	2	13	14	7284.564	9.3
10	0	10	11,9	9	1	9	10,8	7364.456	16.8
10	0	10	10	9	1	9	9	7364.594	4.1
4	2	3	3	3	1	3	2	7399.262	3.1
4	2	3	5	3	1	3	4	7399.380	-10.0
4	2	2	5	3	1	3	4	7420.698	1.6

4	2	2	4	3	1	3	3	7421.146	-2.4
12	1	11	13,11	11	2	10	12,10	7428.588	-2.0
9	1	9	9	8	0	8	8	7683.502	5.7
9	1	9	10,8	8	0	8	9,7	7683.752	-4.5
7	1	6	8,6	6	0	6	7,5	7770.458	21.1
7	1	6	7	6	0	6	6	7771.004	-0.4
5	2	4	5	4	1	3	4	7806.266	-3.8
5	2	4	6	4	1	3	5	7806.694	-5.9
5	2	4	4	4	1	3	3	7806.820	7.5
5	2	3	5	4	1	3	4	7855.860	-5.7
11	0	11	12,10	10	1	10	11,9	8223.578	6.5
11	0	11	11	10	1	10	10	8223.692	5.1
5	2	4	4	4	1	4	3	8310.290	-7.8
5	2	4	6	4	1	4	5	8310.400	1.2
5	2	4	5	4	1	4	4	8310.792	-6.2
10	1	10	10	9	0	9	9	8347.144	6.2
10	1	10	11,9	9	0	9	10,8	8347.356	-0.2
5	2	3	4	4	1	4	3	8359.758	-3.7
8	2	3	6	4	1	4	5	8359.884	-0.9
5	2	3	5	4	1	4	4	8360.390	-4.1
6	2	5	6	5	1	4	5	8490.942	5.4
6	2	4	6	5	1	4	5	8589.262	-7.1
6	2	4	7,5	5	1	4	6,4	8589.556	-17.3
8	1	7	9,7	7	0	7	8,6	8827.246	7.3
8	1	7	8	7	0	7	7	8827.832	-6.3
11	1	11	11	10	0	10	10	9018.762	0.7
11	1	11	12,10	10	0	10	11,9	9018.948	7.2
12	0	12		11	1	11		9067.974	-6.9
3	3	0		2	2	0		9107.998	4.0
3	3	1		2	2	1		9109.422	-6.0
13	4	10	14,12	13	3	10	14,12	9128.188	-16.1
13	4	9	13	13	3	10	13	9136.914	-8.7
13	4	9	14,12	13	3	10	14,12	9137.026	-6.2
7	2	6	7	6	1	5	6	9151.354	-0.4
7	2	6	8,6	6	1	5	7,5	9151.806	-11.1
12	4	9		12	3	9		9196.698	-9.8
12	4	8		12	3	9		9201.434	25.8
6	2	5	7,5	5	1	5	6,4	9246.540	15.1
6	2	5	6	5	1	5	5	9246.984	6.2
11	4	7		11	3	8		9248.892	20.9
10	4	7		10	3	7		9281.742	5.6
10	4	6		10	3	7		9282.844	2.5
9	4	6		9	3	6		9305.962	10.1
9	4	5		9	3	6		9306.432	5.4
12	4	9		12	3	10		9317.592	10.0

13	4	10		13	3	11		9318.318	1.9
11	4	8		11	3	9		9319.982	-7.0
14	4	11		14	3	12		9323.893	7.2
10	4	7		10	3	8		9324.170	29.3
10	4	6		10	3	8		9325.252	6.2
7	2	5	7	6	1	5	6	9326.080	7.9
7	2	5	8,6	6	1	5	7,5	9326.294	-18.5
13	4	9		13	3	11		9327.156	9.5
9	4	6		9	3	7		9328.972	19.6
9	4	5		9	3	7		9329.456	28.8
6	2	4	5	5	1	5	4	9344.618	-15.4
6	2	4	7	5	1	5	6	9344.738	-4.4
6	2	4	6	5	1	5	5	9345.306	-4.3
14	1	13	15,13	13	2	12	14,12	9498.916	17.9
14	1	13	14	13	2	12	13	9499.190	6.6
12	1	12	12	11	0	11	11	9700.752	1.5
12	1	12	13,11	11	0	11	12,10	9700.904	13.3
8	2	7	8	7	1	6	7	9788.482	12.6
8	2	7	9,7	7	1	6	8,6	9788.930	8.2
4	3	2		3	2	1		9915.666	2.5
4	3	1		3	2	1		9915.842	1.8
4	3	2		3	2	2		9922.790	1.4
4	3	1		3	2	2		9922.976	10.8
9	1	8	10,8	8	0	8	9,7	9928.778	1.1
9	1	8	9	8	0	8	8	9929.420	12.4
7	2	6	8,6	6	1	6	7,5	10207.984	8.3
7	2	6	7	6	1	6	6	10208.426	-5.9
7	2	5	8,6	6	1	6	7,5	10382.512	40.9
7	2	5	7	6	1	6	6	10383.148	-1.5
13	1	13	13	12	0	12	12	10394.150	0.1
13	1	13	14,12	12	0	12	13,11	10394.280	15.3
9	2	8	9	8	1	7	8	10403.648	11.0
9	2	8	10,8	8	1	7	9,7	10404.046	-32.2
14	0	14		13	1	13		10714.786	-7.7
5	3	3		4	2	2		10717.802	-14.0
5	3	2		4	2	2		10718.520	-2.0
5	3	3		4	2	3		10739.148	8.2
5	3	2		4	2	3		10739.852	6.2
9	2	7	9	8	1	7	8	10842.182	13.7
9	2	7	10,8	8	1	7	9,7	10842.282	5.3
10	2	9	10	9	1	8	9	10998.714	-0.5
10	1	9	11,9	9	0	9	10,8	11077.006	2.9
14	1	14		13	0	13		11098.970	21.7
8	2	7	9,7	7	1	7	8,6	11194.778	4.2
8	2	7	8	7	1	7	7	11195.228	-4.8

8	2	6	9,7	7	1	7	8,6	11480.432	8.1
8	2	6	8	7	1	7	7	11481.168	7.5
6	3	4	6	5	2	3	5	11510.490	15.6
6	3	4	7,5	5	2	3	6,4	11510.584	4.7
6	3	3	7,5	5	2	3	6,4	11512.686	-6.2
15	0	15		14	1	14		11520.034	-26.0
6	3	3		5	2	4		11562.172	-2.4
11	2	10	11	10	1	9	10	11576.158	3.2
10	2	8		9	1	8		11636.702	49.4
15	1	15		14	0	14		11814.162	-2.6
13	5	9		13	4	10		11970.778	43.7
12	5	8		12	4	9		11982.050	49.0
7	5	3		7	4	4		12011.314	14.2
6	5	2		6	4	3		12013.322	7.2
5	5	1		5	4	2		12014.536	-41.0
12	2	11	12	11	1	10	11	12139.098	13.6
9	2	8	8	8	1	8	7	12206.852	-15.0
9	2	8	10	8	1	8	9	12206.928	6.5
9	2	8	9	8	1	8	8	12207.340	-15.3
11	1	10	12,10	10	0	10	11,9	12271.886	-31.9
7	3	5	7	6	2	4	6	12289.074	0.5
7	3	5	8,6	6	2	4	7,5	12289.216	7.4
7	3	4	7	6	2	4	6	12294.350	-4.6
7	3	4	8,6	6	2	4	7,5	12294.482	2.6
7	3	5		6	2	5		12387.380	-3.0
7	3	4		6	2	5		12392.602	-55.3
11	2	9		10	1	9		12464.020	-7.0
4	4	0		3	3	1		12589.844	5.2
9	2	7	10,8	8	1	8	9,7	12645.076	-16.6
9	2	7	9	8	1	8	8	12645.878	-8.6
13	2	12	14,12	12	1	11	13,11	12691.718	3.0
8	3	6	8	7	2	5	7	13048.462	27.0
8	3	6	9,7	7	2	5	8,6	13048.606	1.5
8	3	5	8	7	2	5	7	13059.976	-31.5
8	3	5	9,7	7	2	5	8,6	13060.148	-11.5
8	3	5		7	2	6		13234.678	-0.3
14	2	13	15,13	13	1	12	14,12	13237.786	-0.6
10	2	9	10	9	1	9	9	13244.640	14.2
12	2	10	13,11	11	1	10	12,10	13329.600	-32.4
12	2	10	12	11	1	10	11	13329.680	-33.7
12	1	11	11	11	0	11	10	13511.152	-52.5
12	1	11	13	11	0	11	12	13511.292	29.6
12	1	11	12	11	0	11	11	13511.952	29.0
9	3	6	9	8	2	6	8	13806.534	17.6
9	3	6	10,8	8	2	6	9,7	13806.716	21.2

10	2	8	11,9	9	1	9	10,8	13881.684	-3.2
10	2	8	10	9	1	9	9	13882.556	20.6
9	3	6	10,8	8	2	6	9,7	14092.306	-38.8
9	3	6	9	8	2	6	8	14092.388	-56.0
6	4	3		5	3	2		14210.910	-35.1
6	4	2		5	3	3		14211.662	-5.8
11	6	6		11	5	7		14672.198	-5.4
10	6	5		10	5	6		14676.314	5.0
9	6	4		9	5	5		14679.348	-33.9
8	6	3		8	5	4		14681.615	2.5
6	6	1		6	5	2		14684.186	-0.5
10	3	8		9	2	8		14928.320	6.7
7	4	4		6	3	3		15020.116	53.4
7	4	3		6	3	4		15022.250	11.5
11	3	8	12,10	10	2	8	11,9	15237.910	-31.7
5	5	0		4	4	1		16070.762	22.5
9	4	5		8	3	5		16631.444	18.5
9	4	6		8	3	6		16642.504	-7.6
9	4	5		8	3	6		16642.986	-0.4
6	5	1		5	4	2		16881.762	16.1
16	7	10		16	6	11		17321.347	-23.6
15	7	9		15	6	10		17328.855	-12.3
14	7	8		14	6	9		17335.013	-11.1
13	7	7		13	6	8		17340.004	-9.1
12	7	6		12	6	7		17343.986	-7.4
11	7	5		11	6	6		17347.107	-4.6
10	7	4		10	6	5		17349.500	-2.1
9	7	3		9	6	4		17351.290	2.3
8	7	2		8	6	3		17352.579	-0.2
7	7	1		7	6	2		17353.520	43.0
10	4	7		9	3	6		17429.780	18.9
10	4	6		9	3	6		17430.885	18.9
10	4	7		9	3	7		17452.745	-16.6
10	4	6		9	3	7		17453.860	-6.6
7	5	2		6	4	3		17692.554	-18.7
11	4	8		10	3	7		18221.320	12.7
11	4	7		10	3	7		18223.683	15.5
11	4	8		10	3	8		18263.700	-11.6
11	4	7		10	3	8		18266.064	-7.8

[a]More than one listed *F* quantum number indicates a blend.

[b]No listed *F* quantum number indicates that nuclear quadrupole structure is not resolved for this transition.

Table S2. Observed transitions of the singly hydrated complex of conformer E of *p*MPEA.

J'	Ka'	Kc'	F'	J''	Ka''	Kc''	F''	Frequency (MHz)	Obs-calc (kHz)
4	2	3	3	3	1	3	2	6925.164	-9.9
4	2	3	5	3	1	3	4	6925.264	-4.9
4	2	3	4	3	1	3	3	6925.570	2.6
5	2	3	5	4	1	3	4	7323.902	-17.4
5	2	3	6	4	1	3	5	7324.198	-5.6
5	2	3	4	4	1	3	3	7324.296	1.9
9	4	6	9	9	3	6	9	7662.442	-0.9
9	4	6	10,8[a]	9	3	6	10,8	7662.574	-16.7
8	4	5	8	8	3	5	8	7708.926	-3.8
8	4	5	9,7	8	3	5	9,7	7709.076	1.7
7	4	4	7	7	3	4	7	7738.050	-2.8
7	4	4	8,6	7	3	4	8,6	7738.218	11.5
9	4	5	[b]	9	3	7		7752.042	18.5
8	4	4	8	8	3	6	8	7754.020	1.5
8	4	4	9,7	8	3	6	9,7	7754.120	4.6
6	4	3	6	6	3	3	6	7755.390	-0.9
6	4	3	7,5	6	3	3	7,5	7755.548	-23.2
7	4	3	7	7	3	5	7	7758.618	-2.3
7	4	3	8,6	7	3	5	8,6	7758.748	2.2
6	4	2	6	6	3	4	6	7763.634	7.7
6	4	2	7,5	6	3	4	7,5	7763.784	-7.4
5	4	2	5	5	3	2	5	7765.082	-12.1
5	4	2	6,4	5	3	2	6,4	7765.294	-34.5
5	2	4	6,4	4	1	4	5,3	7909.860	15.0
5	2	4	5	4	1	4	4	7910.220	2.0
3	3	0	3	2	2	0	2	8090.988	2.0
3	3	0	4,2	2	2	0	3,1	8091.086	15.9
3	3	1		2	2	1		8094.266	23.4
6	2	4	6	5	1	4	5	8103.622	-14.2
6	2	4	7,5	5	1	4	6,4	8103.852	-13.8
7	1	6	8,6	6	0	6	7,5	8128.104	7.0
7	1	6	7	6	0	6	6	8128.678	-1.3
6	2	5	7,5	5	1	5	6,4	8929.070	0.6
6	2	5	6	5	1	5	5	8929.458	-3.3
4	3	1	4	3	2	1	3	8930.464	-6.0
4	3	1	5,3	3	2	1	4,2	8930.598	-28.0
4	3	2	4	3	2	2	3	8946.294	11.2
4	3	2	5,3	3	2	1	4,2	8946.350	-19.1
8	1	7	9,7	7	0	7	8,6	9339.852	-5.7
8	1	7	8	7	0	7	7	9340.476	0.9
8	2	6		7	1	6		9748.654	13.3
5	3	2	5	4	2	2	4	9758.618	-3.4

5	3	2	6,4	4	2	2	5,3	9758.770	-25.3
5	3	3		4	2	3		9805.032	5.7
16	5	11		16	4	13		9862.778	15.1
15	5	10		15	4	12		9871.702	1.6
14	5	9		14	4	11		9887.296	-24.2
12	5	8		12	4	8		9893.986	33.0
13	5	8		13	4	10		9905.766	-13.7
12	5	7		12	4	9		9924.424	-3.6
11	5	7		11	4	7		9926.286	5.6
11	5	6		11	4	8		9941.589	5.9
10	5	6	10	10	4	6	10	9949.078	3.6
10	5	6	11,9	10	4	6	11,9	9949.182	9.0
10	5	5	10	10	4	7	10	9956.246	-13.0
10	5	5	11,9	10	4	7	11,9	9956.356	5.0
9	5	5	9	9	4	5	9	9965.120	3.2
9	5	5	10,8	9	4	5	10,8	9965.228	1.0
9	5	4	9	9	4	6	9	9968.198	-4.0
9	5	4	10,8	9	4	6	10,8	9968.324	15.1
8	5	4	8	8	4	4	8	9976.168	-22.0
8	5	4	9,7	8	4	4	9,7	9976.316	3.4
8	5	3	8	8	4	5	8	9977.386	8.4
8	5	3	9,7	8	4	5	9,7	9977.532	26.7
7	2	6	8,6	6	1	6	7,5	9982.860	4.5
7	2	6	7	6	1	6	6	9983.258	-2.1
7	5	4	7	7	4	3	7	9983.642	-10.0
7	5	4	8,6	7	4	3	8,6	9983.810	-1.4
7	5	2	8,6	7	4	4	8,6	9984.216	9.4
5	5	0	5	5	4	2	5	9991.476	3.0
5	5	0	6,4	5	4	2	6,4	9991.758	-1.0
17	2	15	17	16	3	13	16	10464.894	2.7
17	2	15	18,16	16	3	13	17,15	10465.022	18.1
6	3	3	6	5	2	3	5	10568.756	-16.3
6	3	3	7,5	5	2	3	6,4	10568.930	-35.1
9	1	8	10,8	8	0	8	9,7	10613.712	-8.6
9	1	8	9	8	0	8	8	10614.358	-2.4
9	2	7		8	1	7		10636.570	-38.8
6	3	4		5	2	4		10673.650	1.5
8	2	7	9,7	7	1	7	8,6	11070.888	13.7
8	2	7	8	7	1	7	7	11071.290	2.5
18	2	16	18	17	3	14	17	11110.808	-18.8
18	2	6	19,17	17	3	14	18,16	11111.008	-1.8
4	4	1		3	3	1		11160.396	44.9
7	3	4	7	6	2	4	6	11354.920	-11.3
7	3	5		6	2	5		11555.852	-7.6
10	2	8	11,9	9	1	8	10,8	11579.782	-10.6

10	2	8	10	9	1	8	9	11579.900	-1.3
10	1	9	11,9	9	0	9	10,8	11943.894	1.4
10	1	9	10	9	0	9	9	11944.548	8.4
5	4	1		4	3	1		12006.516	-9.2
5	4	2		4	3	2		12007.196	11.1
16	6	11	16	16	5	11	16	12069.734	-3.4
16	6	11	17,15	16	5	11	17,15	12069.810	4.8
15	6	10	15	15	5	10	15	12104.918	-38.0
15	6	10	16,14	15	5	10	16,14	12105.030	6.3
8	3	5	8	7	2	5	7	12113.788	2.7
8	3	5	9,7	7	2	5	8,6	12113.962	-55.2
15	6	9	16,14	15	5	11	16,14	12114.660	-9.3
14	6	9	14	14	5	9	14	12132.524	1.2
14	6	9	15,13	14	5	9	15,13	12132.596	3.7
14	6	8	14	14	5	10	14	12137.372	-4.6
14	6	8	15,13	14	5	10	15,13	12137.458	14.7
13	6	8		13	5	8		12154.084	-32.6
13	6	7	13	13	5	9	13	12156.390	13.5
13	6	7	14,12	13	5	9	14,12	12156.454	5.5
12	6	7		12	5	7		12170.838	-34.3
12	6	6		12	5	8		12171.882	-18.8
11	6	6		11	5	6		12183.760	-19.1
11	6	5	11	11	5	7	11	12184.178	33.9
11	6	5	12,10	11	5	7	12,10	12184.260	26.9
9	2	8	9	8	1	8	8	12192.784	-8.8
8	6	2	8	8	5	4	8	12206.036	-29.4
8	6	2	9,7	8	5	4	9,7	12206.210	-3.6
7	6	1	7	7	5	3	7	12209.714	-17.2
7	6	1	8,6	7	6	1	8,6	12209.914	-4.7
6	6	0	6	6	5	2	6	12212.174	12.4
8	3	6		7	2	6		12455.376	-47.3
9	3	6	9	8	2	6	8	12846.588	-4.7
9	3	6	10,8	8	2	6	9,7	12846.802	-31.0
6	4	2		5	3	2		12851.158	-18.2
6	4	3		5	3	3		12853.778	-8.7
11	1	10	11	10	0	10	10	13320.482	-10.3
9	3	7		8	2	7		13376.008	-5.2
10	3	7	11,9	9	2	7	10,8	13560.364	-7.8
12	2	10	13,11	11	1	10	12,10	13657.568	15.8
7	4	3		6	3	3		13692.584	-14.8
7	4	4		6	3	4		13700.340	14.8
5	5	1		4	4	1		14227.877	8.7
13	3	8	12,10	10	2	8	11,9	14266.514	-0.1
8	4	4	8	7	3	4	7	14528.284	36.8
8	4	4	9,7	7	3	4	8,6	14528.352	15.6

8	4	5	8	7	3	5	7	14547.242	-7.8
8	4	5	9,7	7	3	5	8,6	14547.334	23.7
13	2	11	14,12	12	1	11	13,11	14801.932	-23.9
6	5	2		5	4	2		15074.586	35.9
11	3	9	11	10	2	9	10	15293.606	28.4
9	4	5	9	8	3	5	8	15354.786	28.0
9	4	5	10,8	8	3	5	9,7	15354.864	13.7
9	4	6	9	8	3	6	8	15395.630	-11.3
9	4	6	10,8	8	3	6	9,7	15395.630	22.6
8	5	3		7	4	3		16766.092	43.0
8	5	4		7	4	4		16766.466	40.3
11	4	7	11	10	3	7	10	16961.376	25.6
11	4	7	12,10	10	3	7	11,9	16961.500	30.0
6	6	1		5	5	1		17295.197	-16.2
12	4	9		11	3	9		17968.307	-15.7

[a]More than one listed *F* quantum number indicates a blend.

[b]No listed *F* quantum number indicates that nuclear quadrupole structure is not resolved for this transition.

Table S3. A-reduction Hamiltonian parameters of the seven conformers of *p*MPEA.

	Conformer A		Conformer B	
Parameter	Experiment	Calculated	Experiment	Calculated
A (MHz)	2789.7346(9)	2825.6	3624.2597(9)	3675.4
B (MHz)	535.4314(3)	533.3	457.5505(4)	457.1
C (MHz)	509.6128(3)	506.9	428.3959(4)	428.1
Δ_J (kHz)	0.0394(6)		0.0109(6)	
Δ_{JK} (kHz)	-0.168(6)		-0.196(11)	
Δ_K (kHz)	3.01(9)		8.71(14)	
δ_J (kHz)	-0.0037(4)		-0.00052(26)	
δ_K (kHz)	-0.93(12)		-1.25(16)	
X_{aa} (MHz)	-0.083(28)	-0.15	1.597(17)	1.61
X_{bb}-X_{cc} (MHz)	4.389(8)	4.58	5.080(13)	5.80
# of lines	314		313	
rms error (kHz)	18.6		18.4	
μ_A^2/μ^2	0.43	0.59	0.18	0.23
μ_B^2/μ^2	0.23	0.26	0.43	0.33
μ_C^2/μ^2	0.34	0.16	0.39	0.44
Normalized Population	0.10		0.08	

	Conformer C		Conformer D	
Parameter	Experiment	Calculated	Experiment	Calculated
A (MHz)	2740.1288(3)	2756.8	2832.5686(11)	2868.2
B (MHz)	542.18902(13)	541.2	538.3700(4)	535.7
C (MHz)	507.54356(11)	504.8	509.1855(4)	506.9
Δ_J (kHz)	0.04555(27)		0.0349(20)	
Δ_{JK} (kHz)	-0.1702(20)		-0.271(13)	
Δ_K (kHz)	2.726(23)		2.80(12)	
δ_J (kHz)	0.00221(14)		-0.00401(20)	
δ_K (kHz)	0.43(4)		-0.35(6)	
X_{aa} (MHz)	-0.529(12)	-0.51	0.939(13)	1.26
X_{bb}-X_{cc} (MHz)	1.2190(17)	4.92	-0.312(22)	-0.37
# of lines	412		381	
rms error (kHz)	17.6		26.1	
μ_A^2/μ^2	0.27	0.38	0.13	0.14
μ_B^2/μ^2	0.31	0.22	0.66	0.50
μ_C^2/μ^2	0.43	0.40	0.21	0.36
Normalized Population	0.15		0.19	

Parameter	Conformer E		Conformer F	
	Experiment	Calculated	Experiment	Calculated
A (MHz)	2750.5801(4)	2782.3	3661.816(15)	3725.9
B (MHz)	547.18957(13)	544.7	457.9536(28)	457.4
C (MHz)	508.55045(14)	506.1	428.6457(25)	428.4
Δ_J (kHz)	0.04191(29)		--	
Δ_{JK} (kHz)	-0.143(3)		-0.19(8)	
Δ_K (kHz)	2.366(26)		6.4(30)	
δ_J (kHz)	0.00318(16)		0.0016(12)	
δ_K (kHz)	0.24(5)		-3.4(12)	
X_{aa} (MHz)	1.339(22)	1.72	2.45(7)	2.60
X_{bb}-X_{cc} (MHz)	1.060(25)	1.16	-1.65(4)	-2.02
# of lines	324		53	
rms error (kHz)	25.2		20.4	
μ_A^2/μ^2	0.32	0.34	--[a]	0.19
μ_B^2/μ^2	0.32	0.22	--[a]	0.03
μ_C^2/μ^2	0.36	0.44	1	0.78
Normalized Population	0.41		0.06	

[a]Transitions with these selection rules were not detected.

Parameter	Conformer G	
	Experiment	Calculated
A (MHz)	3669.9691(14)	3727.8
B (MHz)	457.7252(7)	457.4
C (MHz)	428.5701(5)	428.4
Δ_J (kHz)	0.0152(23)	
Δ_{JK} (kHz)	-0.199(14)	
Δ_K (kHz)	8.34(18)	
δ_J (kHz)	0.0011(7)	
δ_K (kHz)	-0.53(16)	
X_{aa} (MHz)	2.246(21)	2.35
X_{bb}-X_{cc} (MHz)	-1.504(22)	-1.49
# of lines	144	
rms error (kHz)	19.9	
μ_A^2/μ^2	--[a]	0.05
μ_B^2/μ^2	1	0.82
μ_C^2/μ^2	--[a]	0.12
Normalized Population	0.01	

[a]Transitions with these selection rules were not detected.

Supplementary Material for PCCP