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Supplementary Material

**Analysis of the Complex Quadrupole Hyperfine Patterns for Two Chlorine Nuclei
in the Rotational Spectrum of 2,5-Dichlorothiophene**

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Appendix 1: Cartesian coordinates for DCT (MP2/aug-cc-pVTZ)

Appendix 2: Observed frequencies and residuals of the fit of DCT

Appendix 3: r_0 output

Appendix 4: $r_m^{(1)}$ output

Appendix 1. Cartesian coordinates for the equilibrium geometries of DCT (MP2/aug-cc-pVTZ)

³⁵Cl-³⁵Cl – Parent

Center Number	Atom	Cartesian Coordinates (Angstroms)		
		X	Y	Z
1	C	1.225224	-0.230317	-0.000003
2	C	0.707271	-1.503696	0.000049
3	C	-0.707268	-1.503699	-0.000044
4	C	-1.225226	-0.230321	-0.000002
5	S	-0.000001	0.981044	0.000004
6	H	1.328289	-2.38671	0.000077
7	H	-1.328282	-2.386716	-0.000069
8	Cl (35)	-2.87836	0.215351	0.000003
9	Cl (35)	2.878361	0.215351	-0.000007

Appendix 2. Observed rotational frequencies and residuals from the fits for the three isotopologues of 2,5-dichlorothiophene

Parent - ³⁵Cl-³⁵Cl

J'	Ka'	Kc'	l'	F'	J''	Ka''	Kc''	l''	F''	v _{obs} /MHz	obs-calc
6	1	5	0	6	6	0	6	2	6	5532.7761	-0.0002
6	1	5	3	4	6	0	6	3	4	5533.7400	0.0005
6	1	5	2	7	6	0	6	2	7	5534.8405	0.0015
6	1	5	3	8	6	0	6	3	8	5535.6767	0.0000
6	1	5	2	6	6	0	6	0	6	5536.8902	-0.0001
6	1	5	3	7	6	0	6	3	7	5537.2265	0.0004
1	1	1	3	4	0	0	0	3	3	5686.9728	0.0011
1	1	1	2	2	0	0	0	2	2	5690.1049	-0.0003
1	1	1	2	3	0	0	0	2	2	5690.1753	0.0005
1	1	1	3	3	0	0	0	3	3	5699.6892	-0.0005
7	1	6	1	7	7	0	7	1	7	6010.3215	0.0002
7	1	6	2	6	7	0	7	2	6	6012.0910	-0.0005
7	1	6	2	7	7	0	7	0	7	6013.8743	0.0011
7	1	6	3	8	7	0	7	3	8	6014.1250	-0.0014
8	1	7	2	8	8	0	8	2	8	6583.5734	0.0004
8	1	7	2	7	8	0	8	2	6	6585.1649	-0.0014
8	1	7	2	6	8	0	8	2	6	6585.1756	-0.0037
8	1	7	0	8	8	0	8	0	8	6586.7747	-0.0017
2	1	2	3	4	1	0	1	3	4	7057.7508	-0.0012
2	1	2	3	5	1	0	1	3	4	7070.9415	0.0008
2	1	2	2	3	1	0	1	2	2	7072.5156	0.0049

2	1	2	2	4	1	0	1	2	3	7072.5356	-0.0007
2	1	2	3	3	1	0	1	1	2	7073.2149	0.0014
2	1	2	0	2	1	0	1	2	2	7082.5244	0.0001
2	1	2	2	2	1	0	1	0	1	7084.4327	-0.0002
2	1	2	3	4	1	0	1	3	3	7085.3284	0.0010
7	0	7	3	7	6	1	6	3	6	7127.1102	0.0000
7	0	7	0	7	6	1	6	2	6	7127.6598	0.0006
7	0	7	3	6	6	1	6	3	5	7127.7563	0.0010
7	0	7	3	8	6	1	6	3	7	7127.7924	-0.0008
7	0	7	1	8	6	1	6	1	7	7128.1421	-0.0008
7	0	7	2	8	6	1	6	2	7	7128.2973	-0.0026
7	0	7	2	6	6	1	6	2	5	7128.3074	-0.0001
7	0	7	1	7	6	1	6	1	6	7128.9654	0.0056
9	1	8	2	7	9	0	9	2	7	7261.7283	0.0026
9	1	8	2	8	9	0	9	2	8	7261.7411	0.0042
10	1	9	3	8	10	0	10	3	8	8047.8092	-0.0005
10	1	9	2	8	10	0	10	2	8	8048.2481	-0.0064
3	1	3	3	3	2	0	2	3	2	8393.3009	-0.0004
3	1	3	1	3	2	0	2	1	2	8394.7973	0.0002
3	1	3	0	3	2	0	2	0	2	8395.8991	0.0000
3	1	3	1	4	2	0	2	1	3	8397.2322	0.0005
3	1	3	3	6	2	0	2	3	5	8399.4463	0.0008
3	1	3	2	5	2	0	2	2	4	8400.2450	-0.0006
3	1	3	2	4	2	0	2	2	3	8400.2668	0.0020
3	1	3	3	4	2	0	2	3	3	8403.4371	0.0002
3	1	3	1	2	2	0	2	1	1	8404.5231	-0.0008
3	1	3	2	3	2	0	2	2	2	8404.6312	-0.0009
3	1	3	3	5	2	0	2	3	4	8405.9633	0.0000
8	0	8	3	6	7	1	7	3	5	8860.2248	-0.0017
8	0	8	3	8	7	1	7	3	7	8860.3446	-0.0001
8	0	8	1	7	7	1	7	1	6	8860.4129	-0.0009
8	0	8	0	8	7	1	7	2	7	8860.7374	0.0057
8	0	8	3	7	7	1	7	3	6	8860.7686	0.0004
8	0	8	3	9	7	1	7	3	8	8860.8954	0.0009
8	0	8	1	9	7	1	7	1	8	8860.9960	-0.0006
8	0	8	3	5	7	1	7	3	4	8861.1087	-0.0035
8	0	8	2	7	7	1	7	2	6	8861.1307	0.0049
8	0	8	2	8	7	1	7	0	7	8861.5173	-0.0032
8	0	8	3	10	7	1	7	3	9	8861.6164	-0.0002
4	1	4	3	2	3	0	3	3	1	9667.0716	0.0000
4	1	4	3	3	3	0	3	3	2	9670.5321	0.0000
4	1	4	1	4	3	0	3	1	3	9672.8062	0.0006
4	1	4	0	4	3	0	3	2	3	9672.9146	0.0016

4	1	4	3	4	3	0	3	3	3	9673.8241	0.0000
4	1	4	2	2	3	0	3	2	1	9674.4775	0.0002
4	1	4	1	5	3	0	3	1	4	9674.8337	-0.0020
4	1	4	2	6	3	0	3	2	5	9675.2616	0.0012
4	1	4	2	3	3	0	3	2	2	9675.2868	-0.0055
4	1	4	2	5	3	0	3	2	4	9675.3733	0.0007
4	1	4	3	5	3	0	3	3	4	9675.6064	-0.0012
4	1	4	3	7	3	0	3	3	6	9675.6696	0.0008
4	1	4	1	3	3	0	3	1	2	9676.2813	0.0011
4	1	4	2	4	3	0	3	0	3	9676.4325	0.0001
4	1	4	3	6	3	0	3	3	5	9679.1695	0.0001
4	1	4	3	6	3	0	3	3	5	9679.1704	0.0009
9	0	9	3	8	8	1	8	3	7	10592.3059	0.0029
9	0	9	2	8	8	1	8	2	7	10592.5477	0.0007
9	0	9	1	9	8	1	8	1	8	10592.7808	-0.0002
11	2	9	2	10	11	1	10	2	10	10721.2497	-0.0001
10	2	8	1	10	10	1	9	1	10	10847.6123	-0.0002
10	2	8	3	10	10	1	9	3	10	10849.7653	0.0007
5	1	5	3	3	4	0	4	3	2	10900.2207	-0.0010
5	1	5	3	2	4	0	4	3	1	10901.0947	-0.0014
5	1	5	3	4	4	0	4	3	3	10901.9561	-0.0005
5	1	5	1	5	4	0	4	1	4	10903.0336	-0.0010
5	1	5	0	5	4	0	4	2	4	10903.0676	-0.0034
5	1	5	3	5	4	0	4	3	4	10903.4260	-0.0016
5	1	5	1	6	4	0	4	1	5	10903.7775	-0.0005
5	1	5	3	8	4	0	4	3	7	10904.2403	-0.0002
5	1	5	2	7	4	0	4	2	6	10904.3016	-0.0048
5	1	5	1	4	4	0	4	1	3	10904.6368	-0.0011
5	1	5	2	5	4	0	4	0	4	10905.4642	-0.0008
5	1	5	3	6	4	0	4	3	5	10905.8227	-0.0009
5	1	5	3	7	4	0	4	3	6	10906.2936	0.0013
8	2	6	3	5	8	1	7	3	5	11253.5253	0.0004
8	2	6	1	8	8	1	7	1	8	11253.8938	0.0000
8	2	6	0	8	8	1	7	2	8	11253.8948	0.0004
8	2	6	3	6	8	1	7	3	6	11254.9772	-0.0006
8	2	6	3	6	8	1	7	3	6	11254.9772	-0.0006
8	2	6	2	6	8	1	7	2	6	11255.5940	0.0005
8	2	6	2	6	8	1	7	2	6	11255.5946	0.0011
8	2	6	3	10	8	1	7	3	10	11256.2061	-0.0013
8	2	6	3	10	8	1	7	3	10	11256.2066	-0.0008
8	2	6	1	7	8	1	7	1	7	11257.0545	0.0011
8	2	6	3	8	8	1	7	3	8	11257.2185	-0.0006
8	2	6	2	8	8	1	7	0	8	11257.3476	0.0005

8	2	6	3	9	8	1	7	3	9	11257.5669	0.0002
7	2	5	0	7	7	1	6	0	7	11501.2089	0.0002
7	2	5	1	7	7	1	6	1	7	11501.2089	0.0006
7	2	5	3	10	7	1	6	3	10	11501.5759	0.0007
7	2	5	3	5	7	1	6	3	5	11502.4448	0.0011
7	2	5	3	6	7	1	6	3	6	11503.3291	-0.0021
7	2	5	1	8	7	1	6	1	8	11503.3439	0.0031
7	2	5	2	8	7	1	6	2	8	11503.4349	0.0009
7	2	5	2	6	7	1	6	2	6	11503.5259	0.0001
7	2	5	3	9	7	1	6	3	9	11504.2964	-0.0001
7	2	5	1	6	7	1	6	1	6	11505.2562	-0.0010
7	2	5	3	7	7	1	6	3	7	11505.5173	0.0002
7	2	5	2	7	7	1	6	2	7	11505.7927	0.0000
7	2	5	3	8	7	1	6	3	8	11506.1813	-0.0004
6	2	4	3	3	6	1	5	3	3	11755.6618	-0.0003
6	2	4	1	6	6	1	5	1	6	11756.4954	0.0005
6	2	4	3	4	6	1	5	3	4	11757.9379	0.0002
6	2	4	3	5	6	1	5	3	5	11759.2931	-0.0007
6	2	4	1	7	6	1	5	1	7	11759.5641	0.0003
6	2	4	2	5	6	1	5	2	5	11759.6780	-0.0017
6	2	4	2	7	6	1	5	2	7	11759.7020	0.0031
6	2	4	2	8	6	1	5	2	8	11759.7193	-0.0036
6	2	4	2	4	6	1	5	2	4	11759.7406	-0.0027
6	2	4	3	8	6	1	5	3	8	11760.9245	-0.0001
6	2	4	1	5	6	1	5	1	5	11762.1336	0.0000
6	2	4	3	6	6	1	5	3	6	11762.3987	0.0000
6	2	4	0	6	6	1	5	2	6	11762.8530	-0.0009
6	2	4	3	7	6	1	5	3	7	11763.3776	0.0004
5	2	3	3	2	5	1	4	3	2	12003.0402	-0.0018
5	2	3	1	5	5	1	4	1	5	12004.5034	-0.0011
5	2	3	2	5	5	1	4	0	5	12004.5115	0.0005
5	2	3	3	8	5	1	4	3	8	12005.6251	-0.0003
5	2	3	3	4	5	1	4	3	4	12008.3333	0.0019
5	2	3	1	6	5	1	4	1	6	12008.8716	0.0006
5	2	3	2	6	5	1	4	2	6	12009.1513	-0.0017
5	2	3	2	4	5	1	4	2	4	12009.1689	-0.0032
5	2	3	2	7	5	1	4	2	7	12009.1828	0.0006
5	2	3	3	7	5	1	4	3	7	12011.2775	-0.0006
5	2	3	1	4	5	1	4	1	4	12012.5743	-0.0023
5	2	3	3	5	5	1	4	3	5	12012.8517	-0.0004
5	2	3	0	5	5	1	4	2	5	12013.7950	0.0001
5	2	3	3	6	5	1	4	3	6	12014.6288	-0.0006
6	1	6	3	4	5	0	5	3	3	12088.8325	0.0006

6	1	6	3	3	5	0	5	3	2	12089.3960	-0.0007
6	1	6	3	5	5	0	5	3	4	12090.0920	0.0003
6	1	6	1	6	5	0	5	1	5	12090.5603	-0.0027
6	1	6	0	6	5	0	5	2	5	12090.5763	0.0000
6	1	6	1	6	5	0	5	2	5	12090.5884	0.0004
6	1	6	3	6	5	0	5	3	5	12090.8162	0.0000
6	1	6	1	7	5	0	5	1	6	12090.9467	0.0004
6	1	6	2	5	5	0	5	2	4	12091.2491	-0.0019
6	1	6	1	5	5	0	5	1	4	12091.2491	-0.0022
6	1	6	2	7	5	0	5	2	6	12091.2670	0.0030
6	1	6	2	6	5	0	5	0	5	12091.9147	-0.0001
6	1	6	3	7	5	0	5	3	6	12092.2419	0.0000
6	1	6	3	8	5	0	5	3	7	12092.5829	0.0002
4	2	2	3	1	4	1	3	3	1	12228.2857	-0.0002
4	2	2	3	3	4	1	3	3	2	12228.6482	0.0010
4	2	2	3	4	4	1	3	3	3	12229.2789	0.0024
4	2	2	1	4	4	1	3	1	4	12231.1847	0.0008
4	2	2	3	2	4	1	3	3	2	12232.3827	-0.0010
4	2	2	3	7	4	1	3	3	7	12233.2800	0.0007
4	2	2	3	3	4	1	3	3	3	12236.3288	-0.0003
4	2	2	1	5	4	1	3	1	5	12237.8284	0.0014
4	2	2	2	5	4	1	3	2	5	12238.4844	0.0023
4	2	2	2	6	4	1	3	2	6	12238.5091	0.0017
4	2	2	3	2	4	1	3	3	3	12240.0654	-0.0003
4	2	2	3	5	4	1	3	3	4	12240.1149	0.0005
4	2	2	3	6	4	1	3	3	6	12242.3932	0.0002
4	2	2	3	4	4	1	3	3	4	12243.5461	0.0002
4	2	2	1	3	4	1	3	1	3	12243.6407	-0.0002
4	2	2	2	4	4	1	3	2	4	12245.7489	-0.0009
4	2	2	3	5	4	1	3	3	5	12247.1077	-0.0009
4	2	2	3	4	4	1	3	3	5	12250.5392	-0.0009
4	2	2	3	3	4	1	3	3	4	12250.5988	0.0002
4	2	2	3	7	4	1	3	3	6	12251.0330	0.0017
4	2	2	3	6	4	1	3	3	5	12251.6824	0.0016
10	0	10	3	8	9	1	9	3	7	12312.3565	-0.0004
10	0	10	1	9	9	1	9	1	8	12312.5680	-0.0007
10	0	10	3	9	9	1	9	3	8	12312.8057	0.0016
10	0	10	2	8	9	1	9	2	7	12312.9760	-0.0031
10	0	10	1	10	9	1	9	1	9	12313.1140	-0.0004
3	2	1	1	3	3	1	2	1	3	12423.2589	0.0000
3	2	1	0	3	3	1	2	0	3	12423.3960	0.0006
3	2	1	3	6	3	1	2	3	6	12427.9328	-0.0004
3	2	1	3	3	3	1	2	3	2	12428.8123	0.0005

3	2	1	3	4	3	1	2	1	4	12434.2836	-0.0011
3	2	1	2	4	3	1	2	2	4	12436.1360	-0.0019
3	2	1	2	5	3	1	2	2	5	12436.1969	-0.0008
3	2	1	3	5	3	1	2	3	5	12444.3378	-0.0003
3	2	1	1	2	3	1	2	1	2	12444.9070	0.0001
3	2	1	2	3	3	1	2	2	3	12448.7884	0.0013
3	2	1	1	4	3	1	2	3	4	12450.9893	0.0020
2	2	0	0	2	2	1	1	0	2	12566.1219	-0.0002
2	2	0	3	5	2	1	1	3	5	12578.8080	-0.0004
2	2	0	1	3	2	1	1	1	3	12587.7162	-0.0009
2	2	0	2	3	2	1	1	2	3	12593.3689	-0.0006
2	2	0	2	4	2	1	1	2	4	12595.3176	-0.0002
2	2	0	3	4	2	1	1	3	4	12614.5933	0.0001
2	2	0	2	2	2	1	1	2	2	12619.7954	-0.0007
2	2	1	0	2	2	1	2	0	2	12894.7926	-0.0006
2	2	1	3	5	2	1	2	3	5	12908.0797	0.0008
2	2	1	1	3	2	1	2	1	3	12915.5861	-0.0001
2	2	1	2	3	2	1	2	2	3	12923.2368	-0.0001
2	2	1	2	4	2	1	2	2	4	12923.3202	-0.0016
2	2	1	3	4	2	1	2	3	4	12945.9687	0.0007
2	2	1	2	2	2	1	2	2	2	12951.6212	-0.0007
2	2	1	3	3	2	1	2	3	3	12953.6262	-0.0002
3	2	2	1	3	3	1	3	1	3	13076.8270	-0.0005
3	2	2	0	3	3	1	3	0	3	13077.0333	0.0007
3	2	2	3	6	3	1	3	3	6	13081.9999	0.0006
3	2	2	1	4	3	1	3	1	4	13089.0957	-0.0003
3	2	2	2	4	3	1	3	2	4	13091.0878	0.0040
3	2	2	2	5	3	1	3	2	5	13091.1339	-0.0007
3	2	2	2	2	3	1	3	2	2	13091.2004	0.0001
3	2	2	1	3	3	1	3	3	3	13098.0060	-0.0007
3	2	2	3	4	3	1	3	3	3	13098.0145	0.0006
3	2	2	3	4	3	1	3	3	5	13100.1825	-0.0029
3	2	2	3	5	3	1	3	3	5	13100.2648	0.0005
3	2	2	1	2	3	1	3	1	2	13100.9276	-0.0004
3	2	2	2	3	3	1	3	2	3	13105.2033	-0.0054
3	2	2	0	3	3	1	3	2	3	13105.2165	0.0008
3	2	2	3	4	3	1	3	3	4	13107.6576	-0.0002
7	1	7	3	5	6	0	6	3	4	13242.7982	-0.0008
7	1	7	3	4	6	0	6	3	3	13243.2444	0.0001
7	1	7	3	6	6	0	6	3	5	13243.7510	0.0000
7	1	7	1	7	6	0	6	1	6	13244.0233	-0.0005
7	1	7	0	7	6	0	6	2	6	13244.0303	0.0008
7	1	7	3	7	6	0	6	3	6	13244.0922	-0.0002

7	1	7	1	8	6	0	6	1	7	13244.2077	0.0013
7	1	7	1	6	6	0	6	1	5	13244.2319	-0.0007
7	1	7	2	5	6	0	6	2	4	13244.3782	-0.0036
7	1	7	2	6	6	0	6	2	5	13244.3942	0.0014
7	1	7	2	8	6	0	6	2	7	13244.4108	0.0034
7	1	7	3	10	6	0	6	3	9	13244.5550	-0.0007
7	1	7	3	8	6	0	6	3	7	13245.0329	-0.0007
7	1	7	3	9	6	0	6	3	8	13245.3470	0.0005
4	2	3	0	4	4	1	4	0	4	13307.0574	-0.0002
4	2	3	3	7	4	1	4	3	7	13309.5153	0.0010
4	2	3	1	5	4	1	4	1	5	13314.8813	0.0006
4	2	3	2	5	4	1	4	2	5	13315.6729	0.0002
4	2	3	2	6	4	1	4	2	6	13315.7025	0.0002
4	2	3	2	3	4	1	4	2	3	13315.7381	0.0006
4	2	3	3	6	4	1	4	3	6	13320.3397	-0.0002
4	2	3	3	4	4	1	4	3	4	13321.6928	-0.0023
4	2	3	2	4	4	1	4	2	4	13324.3263	-0.0013
4	2	3	3	5	4	1	4	3	5	13325.9529	-0.0002
5	2	4	1	5	5	1	5	1	5	13591.6326	-0.0001
5	2	4	0	5	5	1	5	0	5	13591.6433	0.0021
5	2	4	3	8	5	1	5	3	8	13593.0420	0.0008
5	2	4	3	4	5	1	5	3	4	13596.5481	-0.0002
5	2	4	1	6	5	1	5	1	6	13597.1818	0.0004
5	2	4	2	7	5	1	5	2	7	13597.5910	0.0019
5	2	4	2	6	5	1	5	2	6	13597.6352	-0.0002
5	2	4	3	7	5	1	5	3	7	13600.3101	0.0007
5	2	4	1	4	5	1	5	1	4	13602.0062	0.0007
5	2	4	3	5	5	1	5	3	5	13602.3808	0.0009
5	2	4	2	5	5	1	5	2	5	13603.5601	-0.0004
5	2	4	3	6	5	1	5	3	6	13604.6187	0.0006
6	2	5	1	6	6	1	6	1	6	13932.9786	-0.0001
6	2	5	0	6	6	1	6	0	6	13932.9810	-0.0007
6	2	5	3	5	6	1	6	3	5	13936.9172	0.0009
6	2	5	1	7	6	1	6	1	7	13937.2130	-0.0008
6	2	5	2	7	6	1	6	2	7	13937.4181	-0.0032
6	2	5	2	8	6	1	6	2	8	13937.4466	0.0009
6	2	5	3	8	6	1	6	3	8	13939.2069	0.0021
6	2	5	1	5	6	1	6	1	5	13940.8322	0.0006
6	2	5	3	6	6	1	6	3	6	13941.2329	-0.0006
6	2	5	2	6	6	1	6	2	6	13941.8838	0.0003
6	2	5	3	7	6	1	6	3	7	13942.6331	0.0000
7	2	6	3	4	7	1	7	3	4	14331.6030	-0.0019
7	2	6	1	7	7	1	7	1	7	14332.3849	0.0000

7	2	6	3	10	7	1	7	3	10	14333.0274	0.0012
7	2	6	3	5	7	1	7	3	5	14334.2775	0.0009
7	2	6	3	6	7	1	7	3	6	14335.6136	0.0005
7	2	6	1	8	7	1	7	1	8	14335.7697	0.0002
7	2	6	3	9	7	1	7	3	9	14337.1341	0.0002
7	2	6	1	6	7	1	7	1	6	14338.6760	0.0008
7	2	6	3	7	7	1	7	3	7	14339.0278	0.0003
7	2	6	2	7	7	1	7	2	7	14339.4135	0.0004
7	2	6	3	8	7	1	7	3	8	14339.9587	-0.0002
8	1	8	3	6	7	0	7	3	5	14371.4832	-0.0010
8	1	8	3	5	7	0	7	3	4	14371.8667	-0.0003
8	1	8	3	7	7	0	7	3	6	14372.2150	0.0000
8	1	8	1	8	7	0	7	1	7	14372.4268	0.0029
8	1	8	2	7	7	0	7	2	6	14372.6030	0.0019
8	1	8	2	8	7	0	7	0	7	14372.7810	-0.0001
9	1	9	3	7	8	0	8	3	6	15484.7432	0.0000
9	1	9	1	8	8	0	8	1	7	15485.3077	-0.0001
9	1	9	2	8	8	0	8	2	7	15485.5626	0.0019
2	2	1	1	2	1	1	0	1	1	15675.9411	-0.0013
2	2	1	0	2	1	1	0	0	1	15681.3838	-0.0013
2	2	1	3	5	1	1	0	3	4	15681.9319	0.0009
2	2	1	2	4	1	1	0	2	3	15687.9846	0.0006
2	2	1	2	3	1	1	0	2	2	15688.0242	0.0015
2	2	1	3	4	1	1	0	3	3	15691.6489	0.0003
2	2	1	3	4	1	1	0	3	3	15691.6491	0.0005
2	2	1	3	3	1	1	0	3	3	15696.5398	0.0013
2	2	1	1	3	1	1	0	3	2	15696.6751	0.0014
2	2	1	3	3	1	1	0	1	2	15701.7322	-0.0002
2	2	1	3	4	1	1	0	3	4	15706.6308	-0.0005
2	2	0	1	2	1	1	1	1	1	15787.9637	-0.0008
2	2	0	3	1	1	1	1	3	2	15788.7639	-0.0026
2	2	0	1	3	1	1	1	1	2	15791.1995	0.0001
2	2	0	0	2	1	1	1	0	1	15792.8172	-0.0013
2	2	0	1	2	1	1	1	3	2	15793.0734	-0.0003
2	2	0	3	5	1	1	1	3	4	15794.5570	0.0021
2	2	0	2	3	1	1	1	2	3	15801.1510	0.0002
2	2	0	2	3	1	1	1	2	2	15801.2182	-0.0021
2	2	0	2	4	1	1	1	2	3	15801.2344	0.0013
2	2	0	3	4	1	1	1	3	3	15806.5590	0.0012
2	2	0	1	3	1	1	1	3	2	15807.8647	0.0009
2	2	0	2	2	1	1	1	2	1	15809.6853	0.0011
2	2	0	3	3	1	1	1	1	2	15815.8278	0.0000
2	2	0	3	4	1	1	1	3	4	15819.2751	-0.0008

10	1	10	3	8	9	0	9	3	7	16592.5574	-0.0051
10	1	10	2	8	9	0	9	2	7	16593.1714	0.0028
3	2	2	3	6	2	1	1	3	5	17066.6269	0.0006
3	2	2	1	4	2	1	1	1	3	17070.6276	-0.0002
3	2	2	2	5	2	1	1	2	4	17073.2263	0.0006
3	2	2	3	5	2	1	1	3	4	17077.8177	-0.0002
3	2	1	3	6	2	1	2	3	5	17408.9747	0.0020
3	2	1	2	4	2	1	2	2	3	17414.3052	0.0005
3	2	1	2	5	2	1	2	2	4	17414.3457	0.0001
3	2	1	2	5	2	1	2	2	4	17414.3462	0.0006
3	2	1	3	5	2	1	2	3	4	17422.3064	0.0002
4	2	3	0	4	3	1	2	0	3	18391.3633	0.0000
4	2	3	3	7	3	1	2	3	6	18393.8457	0.0009
4	2	3	1	5	3	1	2	1	4	18395.8654	0.0001
4	2	3	2	5	3	1	2	2	4	18396.9964	-0.0018
4	2	3	2	6	3	1	2	2	5	18397.0318	0.0009
4	2	3	3	4	3	1	2	3	3	18398.3040	-0.0012
4	2	3	1	3	3	1	2	1	2	18400.8427	0.0004
4	2	3	3	6	3	1	2	3	5	18401.3882	0.0001
4	2	3	2	4	3	1	2	2	3	18402.5785	0.0002
4	2	3	3	5	3	1	2	3	4	18403.4649	0.0003

³⁷Cl-³⁵Cl

J'	Ka'	Kc'	F1'	F'	J''	Ka''	Kc''	F1''	F''	$\nu_{\text{obs}}/\text{MHz}$	obs-calc
1	1	1	1	2	0	0	0	2	3	5660.2697	-0.0008
1	1	1	3	4	0	0	0	2	3	5667.7674	0.0005
1	1	1	2	2	0	0	0	2	2	5670.4483	-0.0001
1	1	1	3	3	0	0	0	2	2	5670.5767	0.0003
1	1	1	3	2	0	0	0	2	1	5675.3996	0.0000
1	1	1	2	3	0	0	0	2	3	5679.1784	-0.0009
7	1	6	9	10	7	0	7	9	10	5934.5287	0.0015
7	1	6	7	8	7	0	7	7	8	5935.6230	-0.0006
7	1	6	8	9	7	0	7	8	9	5935.7404	0.0021
7	1	6	9	8	7	0	7	9	8	5935.9500	0.0004
7	1	6	6	6	7	0	7	6	6	5935.9888	0.0022
7	1	6	9	9	7	0	7	9	9	5936.4473	0.0015
7	1	6	7	7	7	0	7	7	7	5937.3965	0.0003
7	1	6	8	8	7	0	7	8	8	5937.6193	-0.0003
8	1	7	10	8	8	0	8	10	8	6475.9223	-0.0008
8	1	7	7	8	8	0	8	7	8	6475.9655	-0.0002
8	1	7	9	7	8	0	8	9	7	6477.1244	0.0021
8	1	7	8	9	8	0	8	8	9	6477.1419	-0.0039

8	1	7	9	10	8	0	8	9	10	6477.3062	0.0001
8	1	7	10	9	8	0	8	10	9	6477.4522	-0.0024
8	1	7	10	10	8	0	8	10	10	6477.8545	0.0000
7	0	7	8	8	6	1	6	7	7	6835.3888	-0.0010
7	0	7	9	8	6	1	6	8	7	6835.6823	0.0020
7	0	7	7	8	6	1	6	6	7	6835.8497	-0.0007
7	0	7	8	9	6	1	6	7	8	6835.9183	-0.0013
7	0	7	9	9	6	1	6	8	8	6836.2589	0.0021
7	0	7	9	10	6	1	6	8	9	6836.6939	-0.0009
2	1	2	2	2	1	0	1	1	2	7000.2143	-0.0001
2	1	2	2	3	1	0	1	1	2	7002.5648	0.0010
2	1	2	2	1	1	0	1	3	1	7003.0717	-0.0011
2	1	2	3	1	1	0	1	1	1	7003.7695	-0.0003
2	1	2	3	4	1	0	1	3	4	7009.3623	-0.0016
2	1	2	4	2	1	0	1	1	2	7010.2091	0.0001
2	1	2	2	2	1	0	1	1	1	7010.7349	-0.0011
2	1	2	1	2	1	0	1	3	1	7011.3495	0.0012
2	1	2	1	1	1	0	1	1	2	7011.8568	-0.0009
2	1	2	4	2	1	0	1	3	1	7013.0019	0.0000
2	1	2	3	2	1	0	1	2	2	7013.4871	-0.0008
2	1	2	1	2	1	0	1	1	1	7019.0763	-0.0005
2	1	2	4	2	1	0	1	1	1	7020.7295	-0.0010
2	1	2	4	5	1	0	1	3	4	7021.2746	0.0005
2	1	2	4	3	1	0	1	2	2	7022.4165	0.0004
2	1	2	4	3	1	0	1	3	3	7022.5937	-0.0008
2	1	2	4	4	1	0	1	3	3	7022.6956	0.0005
2	1	2	3	3	1	0	1	3	2	7023.6492	-0.0007
2	1	2	1	2	1	0	1	2	2	7030.8854	0.0004
2	1	2	3	3	1	0	1	2	3	7031.7283	-0.0003
2	1	2	3	2	1	0	1	2	1	7033.3543	-0.0011
2	1	2	2	2	1	0	1	3	2	7033.3765	0.0035
2	1	2	3	4	1	0	1	2	3	7034.1263	0.0007
2	1	2	2	3	1	0	1	3	2	7035.7225	0.0001
2	1	2	3	1	1	0	1	2	0	7040.5410	-0.0009
2	1	2	2	2	1	0	1	2	3	7041.4505	-0.0011
2	1	2	2	1	1	0	1	2	1	7042.4763	-0.0008
2	1	2	2	3	1	0	1	2	3	7043.8021	0.0011
9	1	8	8	9	9	0	9	8	9	7114.8788	0.0035
9	1	8	9	10	9	0	9	9	10	7116.0028	-0.0005
9	1	8	8	7	9	0	9	8	7	7116.2286	-0.0030
9	1	8	11	10	9	0	9	11	10	7116.2981	0.0000
9	1	8	8	8	9	0	9	8	8	7116.3552	-0.0015
9	1	8	9	9	9	0	9	9	9	7117.5210	0.0010

9	1	8	10	10	9	0	9	10	10	7117.6943	0.0008
3	1	3	2	2	2	0	2	1	2	8306.6662	0.0006
3	1	3	4	2	2	0	2	1	1	8308.5934	-0.0012
3	1	3	4	3	2	0	2	4	3	8309.9287	-0.0022
3	1	3	4	2	2	0	2	4	2	8311.6967	-0.0001
3	1	3	2	1	2	0	2	1	1	8315.7075	0.0012
3	1	3	3	3	2	0	2	2	2	8316.3922	0.0009
3	1	3	5	3	2	0	2	4	2	8317.4125	0.0010
3	1	3	2	3	2	0	2	1	2	8318.9303	0.0000
3	1	3	3	4	2	0	2	2	3	8320.1158	0.0000
3	1	3	4	4	2	0	2	3	4	8321.1825	-0.0002
3	1	3	5	6	2	0	2	4	5	8321.8625	0.0006
3	1	3	2	2	2	0	2	2	1	8322.2826	-0.0049
3	1	3	5	4	2	0	2	4	3	8322.3022	0.0012
3	1	3	5	5	2	0	2	4	4	8322.5942	0.0002
3	1	3	4	4	2	0	2	3	3	8325.4732	0.0001
3	1	3	3	2	2	0	2	3	1	8326.4816	0.0019
3	1	3	4	3	2	0	2	3	2	8326.5045	-0.0009
3	1	3	4	5	2	0	2	3	4	8327.6612	0.0003
3	1	3	4	2	2	0	2	2	2	8330.2230	0.0000
3	1	3	3	3	2	0	2	3	3	8334.1392	-0.0009
3	1	3	2	2	2	0	2	3	2	8338.8958	0.0013
8	0	8	9	8	7	1	7	8	7	8528.1060	0.0002
8	0	8	8	7	7	1	7	7	6	8528.1674	-0.0011
8	0	8	8	8	7	1	7	7	7	8528.4496	-0.0009
8	0	8	9	9	7	1	7	8	8	8528.5966	0.0001
8	0	8	9	7	7	1	7	8	6	8528.6061	0.0026
8	0	8	7	7	7	1	7	6	6	8528.6618	-0.0042
8	0	8	10	9	7	1	7	9	8	8528.6753	0.0011
8	0	8	7	6	7	1	7	6	5	8528.7275	0.0011
8	0	8	8	9	7	1	7	7	8	8528.7925	-0.0012
8	0	8	9	10	7	1	7	8	9	8528.8575	-0.0021
8	0	8	10	8	7	1	7	9	7	8529.1033	0.0003
8	0	8	10	10	7	1	7	9	9	8529.1769	-0.0006
4	1	4	3	2	3	0	3	2	1	9567.8813	-0.0001
4	1	4	5	3	3	0	3	4	2	9568.2733	0.0000
4	1	4	4	4	3	0	3	3	3	9570.8712	0.0008
4	1	4	6	4	3	0	3	5	3	9571.7202	-0.0011
4	1	4	3	4	3	0	3	2	3	9571.7686	-0.0004
4	1	4	4	5	3	0	3	3	4	9572.0128	0.0000
4	1	4	6	7	3	0	3	5	6	9572.4136	0.0009
4	1	4	3	3	3	0	3	2	2	9572.7900	0.0000
4	1	4	6	5	3	0	3	5	4	9572.9684	0.0005

4	1	4	5	4	3	0	3	4	3	9575.3035	0.0000
4	1	4	6	6	3	0	3	5	5	9575.5440	0.0001
4	1	4	5	5	3	0	3	4	4	9575.7275	0.0004
9	0	9	9	8	8	1	8	8	7	10222.0385	-0.0026
9	0	9	10	9	8	1	8	9	8	10222.0515	0.0021
9	0	9	10	8	8	1	8	9	7	10222.3721	0.0007
9	0	9	8	6	8	1	8	7	5	10222.4137	0.0027
9	0	9	11	10	8	1	8	10	9	10222.4137	-0.0005
9	0	9	11	9	8	1	8	10	8	10222.6846	0.0048
5	1	5	4	3	4	0	4	3	2	10773.6362	0.0001
5	1	5	4	2	4	0	4	3	1	10774.3462	0.0011
5	1	5	6	4	4	0	4	5	3	10775.3529	0.0007
5	1	5	7	5	4	0	4	6	4	10775.9107	0.0008
5	1	5	4	5	4	0	4	3	4	10776.2379	0.0000
5	1	5	5	5	4	0	4	4	4	10776.4279	-0.0012
5	1	5	5	6	4	0	4	4	5	10776.8786	-0.0008
5	1	5	7	6	4	0	4	6	5	10776.9932	0.0027
5	1	5	7	8	4	0	4	6	7	10777.1262	0.0019
5	1	5	6	7	4	0	4	5	6	10777.2315	0.0015
5	1	5	5	4	4	0	4	4	3	10777.5312	-0.0009
5	1	5	6	5	4	0	4	5	4	10778.2296	-0.0004
5	1	5	6	6	4	0	4	5	5	10778.5396	0.0000
5	1	5	7	7	4	0	4	6	6	10778.9040	0.0000
8	2	6	9	10	8	1	7	9	10	11341.5693	-0.0023
8	2	6	7	7	8	1	7	7	7	11341.7953	0.0030
8	2	6	10	9	8	1	7	10	9	11341.7953	-0.0011
8	2	6	10	10	8	1	7	10	10	11342.2135	-0.0005
7	2	5	9	7	7	1	6	9	7	11584.8156	-0.0020
7	2	5	6	7	7	1	6	6	7	11584.8805	-0.0051
7	2	5	9	10	7	1	6	9	10	11585.1740	0.0000
7	2	5	8	9	7	1	6	8	9	11586.7756	0.0002
7	2	5	6	5	7	1	6	6	5	11586.8725	0.0001
7	2	5	9	8	7	1	6	9	8	11586.9627	-0.0004
7	2	5	9	9	7	1	6	9	9	11587.6871	0.0007
7	2	5	7	7	7	1	6	7	7	11588.9507	0.0004
7	2	5	8	8	7	1	6	8	8	11589.2870	0.0001
6	2	4	8	9	6	1	5	8	9	11835.1271	0.0015
6	2	4	6	7	6	1	5	6	7	11837.0663	0.0003
6	2	4	7	8	6	1	5	7	8	11837.3175	0.0000
6	2	4	8	7	6	1	5	8	7	11837.5736	0.0017
6	2	4	8	8	6	1	5	8	8	11838.5701	0.0002
6	2	4	6	6	6	1	5	6	6	11840.2154	-0.0016
6	2	4	7	7	6	1	5	7	7	11840.6757	0.0015

6	1	6	6	4	5	0	5	4	3	11939.4268	0.0005
6	1	6	5	3	5	0	5	4	2	11939.8744	-0.0010
6	1	6	7	5	5	0	5	6	4	11940.6812	0.0012
6	1	6	8	6	5	0	5	7	5	11940.8188	0.0000
6	1	6	5	6	5	0	5	4	5	11941.0175	0.0000
6	1	6	7	6	5	0	5	5	5	11941.1345	-0.0025
6	1	6	5	5	5	0	5	4	4	11941.3201	-0.0012
6	1	6	6	7	5	0	5	5	6	11941.3844	-0.0033
6	1	6	8	7	5	0	5	7	6	11941.4005	0.0007
6	1	6	5	4	5	0	5	5	3	11941.4432	-0.0048
6	1	6	6	5	5	0	5	5	4	11941.5386	0.0021
6	1	6	7	8	5	0	5	6	7	11941.5763	-0.0025
6	1	6	8	9	5	0	5	7	8	11941.5942	0.0021
6	1	6	6	6	5	0	5	6	5	11942.1173	-0.0004
6	1	6	7	7	5	0	5	6	6	11942.4102	-0.0002
6	1	6	8	8	5	0	5	7	7	11942.6590	0.0001
5	2	3	4	2	5	1	4	4	2	12073.8222	0.0004
5	2	3	7	5	5	1	4	7	5	12074.9970	-0.0007
5	2	3	4	5	5	1	4	4	5	12075.2606	0.0003
5	2	3	7	8	5	1	4	7	8	12076.1290	-0.0007
5	2	3	6	4	5	1	4	6	4	12078.2373	0.0000
5	2	3	5	6	5	1	4	5	6	12078.7897	0.0006
5	2	3	6	7	5	1	4	6	7	12079.1977	0.0000
5	2	3	7	6	5	1	4	7	6	12079.5145	0.0040
5	2	3	4	4	5	1	4	4	4	12079.5942	0.0008
5	2	3	7	7	5	1	4	7	7	12081.2804	-0.0003
5	2	3	5	4	5	1	4	5	4	12082.3403	-0.0001
5	2	3	5	5	5	1	4	5	5	12082.5650	0.0001
5	2	3	6	5	5	1	4	6	5	12083.4424	-0.0006
5	2	3	6	6	5	1	4	6	6	12084.1697	-0.0004
4	2	2	6	4	4	1	3	6	4	12293.5816	0.0005
4	2	2	3	4	4	1	3	3	4	12294.0899	0.0002
4	2	2	6	7	4	1	3	6	7	12295.7025	0.0001
4	2	2	4	5	4	1	3	4	5	12299.4883	0.0005
4	2	2	5	6	4	1	3	5	6	12300.2315	-0.0002
4	2	2	6	5	4	1	3	6	5	12300.6210	0.0008
4	2	2	6	6	4	1	3	6	6	12303.9795	0.0000
4	2	2	4	4	4	1	3	4	4	12304.8516	-0.0002
4	2	2	4	3	4	1	3	4	3	12304.9817	0.0019
4	2	2	5	4	4	1	3	5	4	12306.8738	-0.0003
4	2	2	5	5	4	1	3	5	5	12308.0612	0.0003
3	2	1	5	3	3	1	2	5	3	12478.0138	0.0005
3	2	1	2	3	3	1	2	2	3	12479.2160	-0.0008

3	2	1	5	6	3	1	2	5	6	12482.7252	0.0003
3	2	1	3	4	3	1	2	3	4	12488.1802	0.0000
3	2	1	4	5	3	1	2	5	5	12489.9113	0.0004
3	2	1	5	4	3	1	2	5	4	12490.2997	-0.0001
3	2	1	4	2	3	1	2	2	2	12490.4015	0.0000
3	2	1	5	5	3	1	2	4	5	12497.5853	-0.0004
3	2	1	3	2	3	1	2	3	2	12498.0080	0.0007
3	2	1	4	3	3	1	2	4	3	12501.4140	-0.0036
3	2	1	3	3	3	1	2	4	3	12501.4289	-0.0002
3	2	1	4	4	3	1	2	4	4	12503.3544	0.0008
2	2	0	4	5	2	1	1	4	5	12626.4229	-0.0004
2	2	0	2	3	2	1	1	2	3	12631.6131	0.0003
2	2	0	4	3	2	1	1	4	3	12638.5478	-0.0020
2	2	0	4	4	2	1	1	4	4	12638.5619	0.0019
2	2	0	3	4	2	1	1	3	4	12658.7295	-0.0004
2	2	0	3	2	2	1	1	3	2	12663.5989	-0.0005
2	2	1	4	5	2	1	2	4	5	12941.9475	0.0000
2	2	1	2	3	2	1	2	2	3	12948.5582	0.0002
2	2	1	4	4	2	1	2	4	4	12955.2618	0.0004
2	2	1	4	3	2	1	2	4	3	12955.4934	0.0005
2	2	1	3	4	2	1	2	3	4	12976.1315	-0.0003
2	2	1	3	2	2	1	2	3	2	12981.0024	0.0002
7	1	7	7	5	6	0	6	6	4	13071.2592	0.0003
7	1	7	6	4	6	0	6	5	3	13071.6014	-0.0002
7	1	7	8	6	6	0	6	7	5	13072.1802	0.0019
7	1	7	9	7	6	0	6	8	6	13072.2270	-0.0022
7	1	7	8	7	6	0	6	7	6	13072.3486	-0.0018
7	1	7	6	7	6	0	6	5	6	13072.3661	0.0019
7	1	7	7	6	6	0	6	6	5	13072.4817	0.0019
7	1	7	9	8	6	0	6	8	7	13072.5212	-0.0035
7	1	7	6	5	6	0	6	5	4	13072.5493	-0.0013
7	1	7	7	8	6	0	6	6	7	13072.5635	0.0029
7	1	7	8	9	6	0	6	7	8	13072.6796	0.0000
7	1	7	9	10	6	0	6	8	9	13072.7693	0.0003
7	1	7	7	7	6	0	6	6	6	13072.9409	-0.0012
7	1	7	8	8	6	0	6	7	7	13073.1907	-0.0001
7	1	7	9	9	6	0	6	8	8	13073.4133	0.0002
3	2	2	5	3	3	1	3	5	3	13102.3106	-0.0029
3	2	2	3	3	3	1	3	2	3	13103.6057	0.0008
3	2	2	5	6	3	1	3	5	6	13107.4846	0.0011
3	2	2	5	4	3	1	3	3	4	13113.5343	0.0014
3	2	2	4	5	3	1	3	5	5	13115.4266	0.0008
3	2	2	3	4	3	1	3	5	4	13115.8821	0.0000

3	2	2	2	2	3	1	3	2	2	13116.0175	-0.0017
3	2	2	4	4	3	1	3	3	3	13121.7766	0.0009
3	2	2	4	4	3	1	3	4	5	13123.9631	-0.0015
3	2	2	5	5	3	1	3	4	5	13124.0295	0.0003
3	2	2	3	2	3	1	3	3	2	13124.4932	-0.0007
3	2	2	4	3	3	1	3	4	3	13128.3011	-0.0008
3	2	2	4	4	3	1	3	4	4	13130.4423	-0.0004
4	2	3	6	4	4	1	4	6	4	13321.7733	0.0007
4	2	3	3	4	4	1	4	3	4	13322.3968	0.0003
4	2	3	6	7	4	1	4	6	7	13324.2994	-0.0010
4	2	3	5	3	4	1	4	5	3	13327.0850	-0.0024
4	2	3	4	5	4	1	4	4	5	13328.7603	0.0009
4	2	3	5	6	4	1	4	5	6	13329.6568	0.0005
4	2	3	4	2	4	1	4	4	2	13329.9089	0.0007
4	2	3	6	5	4	1	4	6	5	13330.1403	0.0004
4	2	3	3	3	4	1	4	3	3	13330.2722	0.0000
4	2	3	6	6	4	1	4	6	6	13334.1515	0.0005
4	2	3	4	4	4	1	4	4	4	13335.1628	0.0000
4	2	3	4	3	4	1	4	4	3	13335.3034	-0.0055
4	2	3	5	4	4	1	4	5	4	13337.5856	0.0008
4	2	3	5	5	4	1	4	5	5	13339.0032	0.0010
5	2	4	4	2	5	1	5	4	2	13591.6323	0.0060
5	2	4	7	5	5	1	5	7	5	13593.1220	0.0000
5	2	4	4	5	5	1	5	4	5	13593.4690	-0.0005
5	2	4	7	8	5	1	5	7	8	13594.5684	-0.0010
5	2	4	4	3	5	1	5	4	3	13595.0413	-0.0021
5	2	4	5	6	5	1	5	5	6	13597.9593	0.0001
5	2	4	6	7	5	1	5	6	7	13598.4885	0.0006
5	2	4	7	6	5	1	5	7	6	13598.9463	0.0008
5	2	4	7	7	5	1	5	7	7	13601.2138	0.0007
5	2	4	6	5	5	1	5	6	5	13603.9911	-0.0002
5	2	4	6	6	5	1	5	6	6	13604.9221	0.0003
8	1	8	8	6	7	0	7	7	5	14177.6401	-0.0019
8	1	8	8	7	7	0	7	7	6	14178.3776	0.0063
8	1	8	10	8	7	0	7	9	7	14178.3776	0.0009
8	1	8	7	8	7	0	7	6	7	14178.4708	-0.0038
8	1	8	7	7	7	0	7	6	6	14178.4858	0.0026
8	1	8	8	9	7	0	7	7	8	14178.5575	-0.0019
8	1	8	9	10	7	0	7	8	9	14178.6379	-0.0019
8	1	8	9	9	7	0	7	8	8	14178.9397	0.0002
8	1	8	10	10	7	0	7	9	9	14179.1560	-0.0011
9	1	9	10	9	8	0	8	9	8	15268.1197	0.0024
9	1	9	10	8	8	0	8	9	7	15268.1692	-0.0006

9	1	9	8	9	8	0	8	7	8	15268.3101	-0.0040
9	1	9	9	10	8	0	8	8	9	15268.3320	0.0026
9	1	9	9	9	8	0	8	8	8	15268.3734	-0.0037
9	1	9	10	10	8	0	8	9	9	15268.5482	0.0025
2	2	1	1	1	1	1	0	1	2	15650.2843	-0.0022
2	2	1	4	5	1	1	0	3	4	15654.2458	0.0001
2	2	1	4	4	1	1	0	3	3	15659.5311	0.0014
2	2	1	4	3	1	1	0	2	2	15659.8461	0.0009
2	2	1	3	4	1	1	0	2	3	15663.0691	0.0000
2	2	1	3	2	1	1	0	2	1	15665.6822	0.0000
2	2	1	3	3	1	1	0	2	3	15667.3174	0.0003
2	2	1	2	3	1	1	0	1	2	15667.4324	0.0020
2	2	1	3	3	1	1	0	3	2	15671.7880	-0.0009
2	2	1	2	2	1	1	0	1	2	15671.8022	0.0016
2	2	1	3	4	1	1	0	3	4	15676.5183	-0.0015
2	2	0	1	1	1	1	1	1	2	15756.3654	-0.0020
2	2	0	2	3	1	1	1	3	2	15758.3969	0.0009
2	2	0	4	5	1	1	1	3	4	15761.6494	0.0010
2	2	0	4	4	1	1	1	3	3	15767.4726	0.0015
2	2	0	4	3	1	1	1	2	2	15767.7296	-0.0005
2	2	0	3	4	1	1	1	2	3	15772.5286	0.0006
2	2	0	2	3	1	1	1	1	2	15773.5251	0.0001
2	2	0	3	2	1	1	1	2	1	15775.2247	0.0011
2	2	0	3	3	1	1	1	2	3	15776.7777	-0.0014
2	2	0	2	1	1	1	1	3	1	15776.7980	0.0003
2	2	0	3	3	1	1	1	3	2	15780.5587	-0.0001
2	2	0	3	4	1	1	1	3	4	15783.9390	-0.0015
3	2	1	5	6	2	1	2	4	5	17334.6383	0.0019
3	2	1	3	4	2	1	2	2	3	17336.9163	0.0007
3	2	1	4	5	2	1	2	4	4	17339.3242	0.0012
3	2	1	5	5	2	1	2	3	4	17346.6852	0.0011
3	2	1	4	4	2	1	2	3	3	17349.0442	0.0008
4	2	3	6	4	3	1	2	5	3	18305.1990	0.0002
4	2	3	3	4	3	1	2	2	3	18305.8938	0.0003
4	2	3	6	7	3	1	2	5	6	18307.8263	0.0004
4	2	3	4	5	3	1	2	3	4	18309.6327	0.0001
4	2	3	5	6	3	1	2	5	5	18310.6168	-0.0012
4	2	3	6	5	3	1	2	5	4	18310.6327	0.0019
4	2	3	4	4	3	1	2	3	3	18311.8074	-0.0005
4	2	3	4	3	3	1	2	3	2	18314.1307	0.0003
4	2	3	6	6	3	1	2	4	5	18314.6185	0.0012
4	2	3	5	4	3	1	2	4	3	18315.6532	0.0000

³⁷Cl-³⁷Cl

J'	Ka'	Kc'	l'	F'	J''	Ka''	Kc''	l''	F''	v _{obs} /MHz	obs-calc
1	1	1	3	4	0	0	0	3	3	5648.6942	0.0001
1	1	1	2	3	0	0	0	2	2	5651.2120	-0.0016
2	1	2	3	5	1	0	1	3	4	6972.3026	0.0010
2	1	2	2	4	1	0	1	2	3	6973.5570	0.0015
2	1	2	3	4	1	0	1	3	3	6983.6242	-0.0008
3	1	3	3	3	2	0	2	3	2	8240.5770	0.0006
3	1	3	1	3	2	0	2	1	2	8241.7517	-0.0007
3	1	3	1	4	2	0	2	1	3	8243.6900	0.0007
3	1	3	3	6	2	0	2	3	5	8245.4285	0.0003
3	1	3	2	5	2	0	2	2	4	8246.0507	-0.0018
3	1	3	2	4	2	0	2	2	3	8246.0643	0.0030
3	1	3	2	2	2	0	2	2	1	8246.0793	-0.0042
3	1	3	3	4	2	0	2	3	3	8248.5606	-0.0003
3	1	3	1	2	2	0	2	1	1	8249.4268	0.0000
3	1	3	3	5	2	0	2	3	4	8250.5590	0.0009
4	1	4	3	7	3	0	3	3	6	9470.6810	0.0014
4	1	4	2	5	3	0	3	2	4	9471.0760	0.0024
4	1	4	3	5	3	0	3	3	4	9473.1006	0.0005
4	1	4	3	6	3	0	3	3	5	9473.4325	-0.0011
9	0	9	2	7	8	1	8	2	6	9859.6109	0.0020
9	0	9	2	8	8	1	8	2	7	9859.6109	0.0018
5	1	5	1	5	4	0	4	1	4	10650.9279	0.0007
5	1	5	0	5	4	0	4	2	4	10650.9549	-0.0013
5	1	5	3	5	4	0	4	3	4	10651.2493	-0.0024
5	1	5	1	6	4	0	4	1	5	10651.4951	0.0000
5	1	5	3	8	4	0	4	3	7	10651.8601	0.0000
5	1	5	2	7	4	0	4	2	6	10651.9096	-0.0010
5	1	5	1	4	4	0	4	1	3	10652.2013	-0.0008
5	1	5	2	5	4	0	4	0	4	10652.8343	-0.0005
5	1	5	3	6	4	0	4	3	5	10653.1050	0.0000
5	1	5	3	7	4	0	4	3	6	10653.4708	-0.0015
6	1	6	1	6	5	0	5	1	5	11793.4499	-0.0030
6	1	6	0	6	5	0	5	2	5	11793.4639	0.0004
6	1	6	3	6	5	0	5	3	5	11793.6453	0.0000
6	1	6	1	7	5	0	5	1	6	11793.7502	0.0009
6	1	6	2	8	5	0	5	2	7	11793.9887	-0.0013
6	1	6	2	7	5	0	5	2	6	11794.0048	0.0043
6	1	6	2	6	5	0	5	0	5	11794.5115	0.0006
6	1	6	3	7	5	0	5	3	6	11794.7694	0.0005
6	1	6	3	8	5	0	5	3	7	11795.0356	0.0002
6	2	4	1	6	6	1	5	1	6	11909.9786	-0.0002

6	2	4	3	9	6	1	5	3	9	11910.5003	0.0005
6	2	4	1	7	6	1	5	1	7	11912.3718	-0.0005
6	2	4	3	8	6	1	5	3	8	11913.4641	-0.0004
5	2	3	0	5	5	1	4	0	5	12143.1453	0.0001
5	2	3	3	8	5	1	4	3	8	12144.0243	0.0005
5	2	3	1	6	5	1	4	1	6	12146.5734	-0.0002
5	2	3	2	7	5	1	4	2	7	12146.8191	0.0020
5	2	3	2	5	5	1	4	2	5	12150.4499	-0.0001
5	2	3	3	6	5	1	4	3	6	12151.1083	0.0000
4	2	2	3	7	4	1	3	3	7	12355.6750	0.0007
4	2	2	2	6	4	1	3	2	6	12359.7869	0.0003
4	2	2	3	6	4	1	3	3	6	12362.8480	0.0005
3	2	1	3	6	3	1	2	3	6	12535.3452	-0.0024
3	2	1	2	4	3	1	2	2	4	12541.8117	0.0012
3	2	1	2	5	3	1	2	2	5	12541.8475	-0.0017
3	2	1	3	5	3	1	2	3	5	12548.2806	0.0003
2	2	0	3	5	2	1	1	3	5	12673.6040	-0.0007
2	2	0	1	3	2	1	1	1	3	12678.9342	-0.0013
2	2	0	2	4	2	1	1	2	4	12684.8048	0.0036
2	2	0	3	4	2	1	1	3	4	12701.9134	0.0011
7	1	7	3	5	6	0	6	3	4	12902.1875	0.0021
7	1	7	1	7	6	0	6	1	6	12903.1565	0.0016
7	1	7	3	7	6	0	6	3	6	12903.1974	-0.0009
7	1	7	1	8	6	0	6	1	7	12903.2913	0.0000
7	1	7	2	9	6	0	6	2	8	12903.4400	-0.0016
7	1	7	3	10	6	0	6	3	9	12903.5709	0.0005
7	1	7	3	8	6	0	6	3	7	12903.9417	0.0009
7	1	7	3	9	6	0	6	3	8	12904.1876	0.0009
2	2	1	2	3	2	1	2	2	3	12986.4818	0.0006
2	2	1	2	4	2	1	2	2	4	12986.5346	-0.0014
3	2	2	3	6	3	1	3	3	6	13132.0353	-0.0001
3	2	2	1	4	3	1	3	1	4	13137.6333	0.0014
3	2	2	2	5	3	1	3	2	5	13139.2311	0.0022
3	2	2	3	5	3	1	3	3	5	13146.4228	0.0000
4	2	3	3	7	4	1	4	3	7	13338.6333	0.0008
4	2	3	1	5	4	1	4	1	5	13342.8622	0.0001
4	2	3	2	5	4	1	4	2	5	13343.4840	-0.0018
4	2	3	2	6	4	1	4	2	6	13343.5081	0.0028
4	2	3	3	6	4	1	4	3	6	13347.1576	-0.0010
5	2	4	3	8	5	1	5	3	8	13596.2469	0.0000
5	2	4	1	6	5	1	5	1	6	13599.5085	-0.0008
5	2	4	2	7	5	1	5	2	7	13599.8237	-0.0041
6	2	5	1	6	6	1	6	1	6	13905.2393	-0.0001

6	2	5	2	8	6	1	6	2	8	13908.7583	0.0008
8	1	8	2	10	7	0	7	2	9	13987.6695	-0.0047
8	1	8	3	10	7	0	7	3	9	13988.2295	-0.0018
2	2	1	3	5	1	1	0	3	4	15626.3996	-0.0002
2	2	1	2	4	1	1	0	2	3	15631.1860	0.0003
2	2	1	3	4	1	1	0	3	3	15634.0626	-0.0004
2	2	0	2	4	1	1	1	2	3	15734.0960	0.0022
2	2	0	3	4	1	1	1	3	3	15738.2836	-0.0012
3	2	2	3	6	2	1	1	3	5	16949.8528	-0.0006
3	2	2	1	4	2	1	1	1	3	16951.3172	0.0004
3	2	2	2	5	2	1	1	2	4	16953.2466	0.0013
3	2	2	2	4	2	1	1	2	3	16953.2839	-0.0009
3	2	2	3	4	2	1	1	3	4	16958.7200	-0.0019
3	2	2	3	5	2	1	1	3	4	16958.7727	0.0009
3	2	1	0	3	2	1	2	0	2	17257.8316	0.0001
3	2	1	3	6	2	1	2	3	5	17261.5158	-0.0007
3	2	1	2	4	2	1	2	2	3	17265.7176	-0.0014
3	2	1	2	5	2	1	2	2	4	17265.7438	0.0003
3	2	1	3	5	2	1	2	3	4	17272.0410	-0.0001
3	2	1	1	4	2	1	2	3	3	17274.1781	-0.0012
4	2	3	0	4	3	1	2	0	3	18220.6980	0.0010
4	2	3	3	7	3	1	2	3	6	18222.6541	0.0017
4	2	3	2	5	3	1	2	2	4	18225.1371	-0.0008
4	2	3	2	6	3	1	2	2	5	18225.1619	0.0008

³⁴S (³⁵Cl-³⁵Cl)

J'	Ka'	Kc'	l'	F'	J''	Ka''	Kc''	l''	F''	v _{obs} /MHz	obs-calc
1	1	1	3	4	0	0	0	3	3	5592.9820	-0.0004
2	1	2	3	5	1	0	1	3	4	6973.3884	0.0007
2	1	2	2	4	1	0	1	2	3	6974.9835	0.0002
2	1	2	3	4	1	0	1	3	3	6987.7743	0.0019
3	1	3	1	3	2	0	2	1	2	8292.8328	0.0007
3	1	3	1	4	2	0	2	1	3	8295.2652	0.0007
3	1	3	3	6	2	0	2	3	5	8297.4765	-0.0008
3	1	3	2	5	2	0	2	2	4	8298.2770	-0.0018
3	1	3	2	3	2	0	2	2	2	8302.6664	0.0000
3	1	3	3	5	2	0	2	3	4	8303.9960	0.0014
4	1	4	2	6	3	0	3	2	5	9568.6591	-0.0022
4	1	4	1	5	3	0	3	1	4	9567.7950	0.0002
4	1	4	3	7	3	0	3	3	6	9568.5920	0.0033
5	1	5	3	4	4	0	4	3	3	10789.4027	0.0000
5	1	5	1	5	4	0	4	1	4	10790.4603	-0.0011

5	1	5	1	6	4	0	4	1	5	10791.1333	-0.0032
5	1	5	3	8	4	0	4	3	7	10791.5978	-0.0006
5	1	5	2	7	4	0	4	2	6	10791.6685	0.0021
5	1	5	3	6	4	0	4	3	5	10793.1872	0.0012
5	1	5	3	7	4	0	4	3	6	10793.6501	-0.0009
6	1	6	1	7	5	0	5	1	6	11972.6282	0.0011
6	1	6	2	8	5	0	5	2	7	11972.9295	-0.0019
6	1	6	2	7	5	0	5	2	6	11972.9477	0.0032
6	1	6	3	8	5	0	5	3	7	11974.2653	0.0011
7	1	7	3	7	6	0	6	3	6	13120.3799	-0.0025
7	1	7	1	8	6	0	6	1	7	13120.4906	-0.0041
7	1	7	3	10	6	0	6	3	9	13120.8415	-0.0004
7	1	7	3	8	6	0	6	3	7	13121.3249	0.0008
7	1	7	3	9	6	0	6	3	8	13121.6343	-0.0010
8	1	8	2	10	7	0	7	2	9	14244.2129	-0.0028
8	1	8	2	9	7	0	7	2	8	14244.2317	0.0012
8	1	8	1	8	7	0	7	1	7	14244.0332	0.0005
5	2	3	3	8	5	1	4	3	8	11722.8617	-0.0033
5	2	3	2	7	5	1	4	2	7	11726.4234	-0.0009
5	2	4	3	8	5	1	5	3	8	13332.9766	-0.0024
5	2	4	1	6	5	1	5	1	6	13337.1156	-0.0036
4	2	2	3	7	4	1	3	3	7	11952.3533	-0.0023
4	2	2	2	6	4	1	3	2	6	11957.5783	-0.0059
4	2	3	3	7	4	1	4	3	7	13044.7313	-0.0010
4	2	3	2	6	4	1	4	2	6	13050.9199	-0.0001
4	2	3	2	5	4	1	4	2	5	13050.8884	-0.0022
3	2	2	3	6	3	1	3	3	6	12813.4865	-0.0029
3	2	2	2	5	3	1	3	2	5	12822.6216	-0.0025
3	2	2	3	5	3	1	3	3	5	12831.7501	-0.0017
3	2	1	3	6	3	1	2	3	6	12149.0084	0.0015
3	2	1	2	5	3	1	2	2	5	12157.2126	-0.0040
3	2	1	2	4	3	1	2	2	4	12157.1648	-0.0013
3	2	1	3	5	3	1	2	3	5	12165.4971	0.0022
2	2	1	2	4	2	1	2	2	4	12652.0439	-0.0003
2	2	1	3	5	2	1	2	3	5	12636.8013	-0.0014
2	2	0	2	4	2	1	1	2	4	12316.7689	-0.0029
2	2	0	3	5	2	1	1	3	5	12301.7874	0.0021

$^{13}\text{C}_\alpha (^{35}\text{Cl}-^{35}\text{Cl})$

J'	Ka'	Kc'	l'	F'	J''	Ka''	Kc''	l''	F''	$\nu_{\text{obs}}/\text{MHz}$	obs-calc
2	1	2	3	5	1	0	1	3	4	7064.1418	-0.0003
2	1	2	2	4	1	0	1	2	3	7065.7354	-0.0026

2	1	2	3	4	1	0	1	3	3	7078.5289	0.0002
3	1	3	1	4	2	0	2	1	3	8387.7812	-0.0010
3	1	3	3	6	2	0	2	3	5	8389.9957	0.0000
3	1	3	2	5	2	0	2	2	4	8390.7932	-0.0028
3	1	3	2	4	2	0	2	2	3	8390.8174	0.0023
3	1	3	3	5	2	0	2	3	4	8396.5153	0.0014
4	1	4	1	5	3	0	3	1	4	9662.9121	0.0005
4	1	4	2	6	3	0	3	2	5	9663.1897	0.0004
4	1	4	2	5	3	0	3	2	4	9663.3559	-0.0020
4	1	4	3	7	3	0	3	3	6	9663.7565	-0.0003
4	1	4	3	6	3	0	3	3	5	9667.2565	-0.0011
5	1	5	3	8	4	0	4	3	7	10890.0177	-0.0039
5	1	5	2	6	4	0	4	2	5	10890.0317	-0.0001
5	1	5	2	7	4	0	4	2	6	10890.0885	0.0010
5	1	5	2	5	4	0	4	0	4	10891.2457	-0.0026
5	1	5	3	6	4	0	4	3	5	10891.6045	-0.0001
5	1	5	3	7	4	0	4	3	6	10892.0710	-0.0024
6	1	6	1	7	5	0	5	1	6	12074.5295	-0.0002
6	1	6	2	8	5	0	5	2	7	12074.8291	-0.0047
6	1	6	2	7	5	0	5	2	6	12074.8496	0.0020
3	2	1	3	6	3	1	2	3	6	12426.5527	0.0003
3	2	1	2	5	3	1	2	2	5	12434.8158	-0.0003
3	2	2	3	6	3	1	3	3	6	13078.1149	0.0017
7	1	7	2	9	6	0	6	2	8	13225.8297	-0.0040
7	1	7	2	8	6	0	6	2	7	13225.8388	-0.0076
7	1	7	3	10	6	0	6	3	9	13225.9952	0.0004
7	1	7	3	9	6	0	6	3	8	13226.7828	-0.0026
4	2	3	3	7	4	1	4	3	7	13304.7429	-0.0006

$^{13}\text{C}_\beta$ (^{35}Cl - ^{35}Cl)

J'	Ka'	Kc'	l'	F'	J''	Ka''	Kc''	l''	F''	$\nu_{\text{obs}}/\text{MHz}$	obs-calc
2	1	2	3	5	1	0	1	3	4	6954.8227	0.0006
2	1	2	2	4	1	0	1	2	3	6956.4148	-0.0028
2	1	2	3	4	1	0	1	3	3	6969.2093	-0.0001
3	1	3	1	4	2	0	2	1	3	8275.0179	0.0028
3	1	3	3	6	2	0	2	3	5	8277.2319	0.0028
3	1	3	2	5	2	0	2	2	4	8278.0297	-0.0007
3	1	3	3	5	2	0	2	3	4	8283.7471	0.0001
4	1	4	1	5	3	0	3	1	4	9545.8149	0.0002
4	1	4	3	7	3	0	3	3	6	9546.6039	-0.0036
4	1	4	2	5	3	0	3	2	4	9546.6907	-0.0022
4	1	4	3	6	3	0	3	3	5	9550.1072	-0.0010

5	1	5	1	6	4	0	4	1	5	10767.3998	-0.0023
5	1	5	3	8	4	0	4	3	7	10767.8597	-0.0050
5	1	5	2	7	4	0	4	2	6	10767.9317	-0.0004
5	1	5	2	6	4	0	4	2	5	10768.0523	-0.0045
5	1	5	3	7	4	0	4	3	6	10769.9169	-0.0002
6	1	6	2	8	5	0	5	2	7	11947.4633	-0.0018
6	1	6	2	7	5	0	5	2	6	11947.4770	-0.0011
6	1	6	3	9	5	0	5	3	8	11947.5373	0.0001
6	1	6	3	7	5	0	5	3	6	11948.4547	-0.0032
6	1	6	3	8	5	0	5	3	7	11948.7936	-0.0045
3	2	1	3	6	3	1	2	3	6	12102.4589	-0.0017
3	2	1	2	5	3	1	2	2	5	12110.6937	0.0007
3	2	2	3	6	3	1	3	3	6	12767.7055	-0.0005
4	2	3	3	7	4	1	4	3	7	12999.2633	-0.0007
7	1	7	2	9	6	0	6	2	8	13093.5482	-0.0048
7	1	7	3	10	6	0	6	3	9	13093.7079	-0.0052
7	1	7	3	9	6	0	6	3	8	13094.5014	-0.0047

Appendix 3: Output from the r_0 structural fit

From A and B rotational constants as an example. For further details of method used, see the SI accompanying reference 12.

NUMBER OF ATOMS = 10 (including 1 dummy atom)
 NO NA NB NC NO.NA NO.NA.NB NO.NA.NB.NC MASS
 1 0 0 0 0.000000 0.000000 0.000000 31.9720710
 2 1 0 0 1.000000 0.000000 0.000000 0.0000010
 3 1 2 0 1.723100 134.674000 0.000000 12.0000000
 4 1 2 3 1.723100 134.674000 180.000000 12.0000000
 5 3 1 2 1.712500 120.189900 0.000000 34.9688527
 6 4 1 2 1.712500 120.189900 0.000000 34.9688527
 7 3 5 2 1.374600 127.278600 180.000000 12.0000000
 8 4 6 2 1.374600 127.278600 180.000000 12.0000000
 9 7 3 1 1.079500 122.774500 -180.000000 1.0078250
 10 8 4 1 1.079500 122.774500 -180.000000 1.0078250

TOTAL NUMBER OF PARAMETERS: 5

Parameters to be fitted:

 R(3, 1) = 1.723100
 , also at atom 4 = 1.723 (difference = 0.000)
 R(5, 3) = 1.712500
 , also at atom 6 = 1.712 (difference = 0.000)
 R(7, 3) = 1.374600
 , also at atom 8 = 1.375 (difference = 0.000)

A(5, 3, 1) = 120.189900
 , also at atom 6 = 120.190 (difference = 0.000)
 A(7, 3, 5) = 127.278600
 , also at atom 8 = 127.279 (difference = 0.000)

FINAL RESULTS OF LEAST SQUARES FIT:

R(3, 1) = 1.716376 +- 0.003839 and at atom 4
 R(5, 3) = 1.711533 +- 0.002121 and at atom 6
 R(7, 3) = 1.376585 +- 0.002149 and at atom 8
 A(5, 3, 1) = 120.524448 +- 0.180645 and at atom 6
 A(7, 3, 5) = 126.207499 +- 0.435240 and at atom 8

Chi-squared = 0.0005153677
 Deviation of fit = 0.008580

Ni Axis	lobs	lcalc	lo-c	Bobs	Bcalc	Bo-c
1 a	101.09691	101.09469	0.00222	4998.9562	4999.0658	-0.1096
1 b	630.00661	629.99718	0.00942	802.1805	802.1925	-0.0120
2 a	101.18587	101.18152	0.00435	4994.5613	4994.7758	-0.2145
2 b	646.29936	646.29579	0.00357	781.9581	781.9624	-0.0043
3 a	101.27795	101.27141	0.00654	4990.0202	4990.3425	-0.3224
3 b	663.01479	663.01747	-0.00267	762.2439	762.2409	0.0031
4 a	102.99675	102.99657	0.00018	4906.7471	4906.7559	-0.0088
4 b	629.99590	629.99718	-0.00129	802.1941	802.1925	0.0016
5 a	101.14762	101.14464	0.00298	4996.4499	4996.5973	-0.1474
5 b	631.47334	631.48225	-0.00891	800.3173	800.3060	0.0113
6 a	103.33674	103.35255	-0.01581	4890.6034	4889.8552	0.7482
6 b	630.51337	630.51343	-0.00007	801.5358	801.5357	0.0001

Correlation coefficients:

	1	2	3	4	5	
1:	R(3, 1)	1.000				
2:	R(5, 3)	-0.878	1.000			
3:	R(7, 3)	-0.665	0.365	1.000		
4:	A(5, 3, 1)	-0.735	0.337	0.909	1.000	
5:	A(7, 3, 5)	0.908	-0.610	-0.694	-0.887	1.000

Final principal coordinates of parent:

ATOM NO.	A	B	C	MASS
1	0.000000	0.982578	0.000000	31.9720710
2	0.000000	1.982578	0.000000	0.0000010
3	1.220547	-0.224158	0.000000	12.0000000
4	-1.220547	-0.224158	0.000000	12.0000000
5	2.875285	0.213090	0.000000	34.9688527
6	-2.875285	0.213090	0.000000	34.9688527
7	0.718130	-1.505784	0.000000	12.0000000
8	-0.718130	-1.505784	0.000000	12.0000000
9	1.349891	-2.381111	0.000000	1.0078250
10	-1.349891	-2.381111	0.000000	1.0078250

Principal coordinates and estimated uncertainties:

ATOM NO.	A	dA	B	dB	C	dC
----------	---	----	---	----	---	----

1	0.00000	0.00000	0.98258	0.00198	0.00000	0.00000
2	0.00000	0.00000	1.98258	0.00198	0.00000	0.00000
3	1.22055	0.00273	-0.22416	0.00335	0.00000	0.00000
4	-1.22055	0.00273	-0.22416	0.00335	0.00000	0.00000
5	2.87529	0.00032	0.21309	0.00192	0.00000	0.00000
6	-2.87529	0.00032	0.21309	0.00192	0.00000	0.00000
7	0.71813	0.00392	-1.50578	0.00111	0.00000	0.00000
8	-0.71813	0.00392	-1.50578	0.00111	0.00000	0.00000
9	1.34989	0.00812	-2.38111	0.00240	0.00000	0.00000
10	-1.34989	0.00812	-2.38111	0.00240	0.00000	0.00000

Appendix 4: Output from the $r_m^{(1)}$ structural fit

NUMBER OF ATOMS = 10 (including 1 dummy atom)

NO	NA	NB	NC	NO.NA	NO.NA.NB	NO.NA.NB.NC	MASS
1	0	0	0	0.000000	0.000000	0.000000	31.9720710
2	1	0	0	1.000000	0.000000	0.000000	0.0000010
3	1	2	0	1.723100	134.674000	0.000000	12.0000000
4	1	2	3	1.723100	134.674000	180.000000	12.0000000
5	3	1	2	1.712500	120.189900	0.000000	34.9688527
6	4	1	2	1.712500	120.189900	0.000000	34.9688527
7	3	5	2	1.374600	127.278600	180.000000	12.0000000
8	4	6	2	1.374600	127.278600	180.000000	12.0000000
9	7	3	1	1.079500	122.774500	-180.000000	1.0078250
10	8	4	1	1.079500	122.774500	-180.000000	1.0078250

TOTAL NUMBER OF PARAMETERS: 8

Parameters to be fitted:

```

-----
R( 3, 1) = 1.723100
           , also at atom 4 = 1.723 (difference = 0.000 )
R( 5, 3) = 1.712500
           , also at atom 6 = 1.712 (difference = 0.000 )
R( 7, 3) = 1.374600
           , also at atom 8 = 1.375 (difference = 0.000 )
A( 5, 3, 1) = 120.189900
              , also at atom 6 = 120.190 (difference = 0.000 )
A( 7, 3, 5) = 127.278600
              , also at atom 8 = 127.279 (difference = 0.000 )
A( 3, 1, 2) = 134.674000
              , also at atom 4 = 134.674 (difference = 0.000 )
c_a = c_b = 0.000000
c_c = 0.000000

```

```

R( 3, 1) = 1.714958 +- 0.003355 and at atom 4
R( 5, 3) = 1.718842 +- 0.001691 and at atom 6
R( 7, 3) = 1.361967 +- 0.004578 and at atom 8
A( 5, 3, 1) = 119.993922 +- 0.252820 and at atom 6

```

A(7, 3, 5) = 126.515029 +- 0.192444 and at atom 8
 A(3, 1, 2) = 134.974674 +- 0.097625 and at atom 4
 c_a = c_b = 0.056615 +- 0.012668
 c_c = 0.076264 +- 0.016455

Chi-squared = 0.0001500365
 Deviation of fit = 0.003873

Ni Axis	lobs	lcalc	lo-c	Bobs	Bcalc	Bo-c
1 a	101.09691	101.09643	0.00048	4998.9562	4998.9798	-0.0237
1 b	630.00661	630.00331	0.00329	802.1805	802.1847	-0.0042
1 c	731.17666	731.17193	0.00473	691.1859	691.1904	-0.0045
2 a	101.18587	101.18436	0.00151	4994.5613	4994.6357	-0.0743
2 b	646.29936	646.29684	0.00252	781.9581	781.9611	-0.0030
2 c	747.55853	747.55786	0.00066	676.0394	676.0400	-0.0006
3 a	101.27795	101.27537	0.00258	4990.0202	4990.1473	-0.1271
3 b	663.01482	663.01302	0.00180	762.2439	762.2460	-0.0021
3 c	764.36620	764.36962	-0.00342	661.1739	661.1710	0.0030
4 a	102.99675	102.99547	0.00128	4906.7471	4906.8081	-0.0610
4 b	629.99590	630.00331	-0.00742	802.1941	802.1847	0.0094
4 c	733.06626	733.06832	-0.00206	689.4043	689.4023	0.0019
5 a	101.14762	101.14992	-0.00230	4996.4499	4996.3361	0.1138
5 b	631.47334	631.47221	0.00113	800.3173	800.3187	-0.0014
5 c	732.69333	732.69466	-0.00133	689.7552	689.7539	0.0013
6 a	103.33674	103.34028	-0.00355	4890.6034	4890.4356	0.1678
6 b	630.51337	630.51476	-0.00139	801.5358	801.5340	0.0018
6 c	733.92574	733.92425	0.00149	688.5969	688.5983	-0.0014

Correlation coefficients:

	1	2	3	4	5	6	7	8	
1:	R(3, 1)	1.000							
2:	R(5, 3)	0.485	1.000						
3:	R(7, 3)	-0.807	-0.873	1.000					
4:	A(5, 3, 1)	-0.900	-0.799	0.977	1.000				
5:	A(7, 3, 5)	0.879	0.463	-0.784	-0.859	1.000			
6:	A(3, 1, 2)	0.805	0.892	-0.986	-0.964	0.729	1.000		
7:	c_a = c_b	-0.764	-0.106	0.340	0.505	-0.459	-0.391	1.000	
8:	c_c	-0.764	-0.106	0.340	0.505	-0.460	-0.391	1.000	1.000

Final principal coordinates of parent:

ATOM NO.	A	B	C	MASS
1	0.000000	0.980469	0.000000	31.9720710
2	0.000000	1.980469	0.000000	0.0000010
3	1.213195	-0.231653	0.000000	12.0000000
4	-1.213195	-0.231653	0.000000	12.0000000
5	2.873224	0.214125	0.000000	34.9688527
6	-2.873224	0.214125	0.000000	34.9688527
7	0.714394	-1.498994	0.000000	12.0000000
8	-0.714394	-1.498994	0.000000	12.0000000
9	1.344967	-2.375178	0.000000	1.0078250
10	-1.344967	-2.375178	0.000000	1.0078250

Principal coordinates and estimated uncertainties:

ATOM NO.	A	dA	B	dB	C	dC
1	0.00000	0.00000	0.98047	0.00088	0.00000	0.00000
2	0.00000	0.00000	1.98047	0.00088	0.00000	0.00000
3	1.21319	0.00141	-0.23165	0.00388	0.00000	0.00000
4	-1.21319	0.00141	-0.23165	0.00388	0.00000	0.00000
5	2.87322	0.00049	0.21413	0.00117	0.00000	0.00000
6	-2.87322	0.00049	0.21413	0.00117	0.00000	0.00000
7	0.71439	0.00224	-1.49899	0.00101	0.00000	0.00000
8	-0.71439	0.00224	-1.49899	0.00101	0.00000	0.00000
9	1.34497	0.00304	-2.37518	0.00121	0.00000	0.00000
10	-1.34497	0.00304	-2.37518	0.00121	0.00000	0.00000