Electronic Supporting Information for

Dispersion-driven conformational preference in the gas phase: microwave spectroscopic and theoretical study of allyl isocyanate

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Appendix I: Equilibrium Structures for the three conformers of allyl-NCO (conf. **I**, **II** and **III**) at the B3LYP-D3(BJ)/cc-pVQZ level of theory.

Appendix II: Basis set benchmark using the B3LYP-D3(BJ) method.

Appendix III: Measured line lists for conf. **III** and conf. **I**, including their parent and minor isotopologues (^{13}C, ^{15}N and ^{18}O).

Appendix IV: Kraitchman coordinates for conf. **I** and conf. **III**.

Appendix I: Equilibrium Structures for the three conformers of allyl-NCO (conf. **I**, **II** and **III**) at the B3LYP-D3(BJ)/cc-pVQZ level of theory.

Table S1. Cartesian coordinates for the equilibrium structure of conf. **I** obtained at the B3LYP-D3(BJ)/cc-pVQZ level of theory.

	Cartesian Coordinates (Angstroms) for conf. I_a		
Atom	X	Y	Z
C1	-1.573008	1.300306	-0.137281
C2	-1.835847	0.041882	0.175177
C3	-0.879272	-1.114169	0.115164
N4	0.445968	-0.789817	-0.338421
C5	1.353678	-0.073413	-0.027790
O6	2.306603	0.576379	0.169988
H7	-2.333303	2.063248	-0.057463
H8	-0.600426	1.616444	-0.486781
H9	-2.828535	-0.235560	0.513095
H10	-1.281362	-1.873757	-0.557266
H11	-0.820308	-1.584809	1.101153
	Cartesian Coordinates (Angstroms) for conf. I_b		
Atom	X	Y	Z
C1	1.573010	1.300305	-0.137280
C2	1.835848	0.041881	0.175177
C3	0.879271	-1.114169	0.115164
N4	-0.445968	-0.789815	-0.338422
C5	-1.353679	-0.073412	-0.027789
O6	-2.306605	0.576379	0.169988
H7	2.333306	2.063246	-0.057463
H8	0.600428	1.616444	-0.486780
H9	2.828535	-0.235562	0.513095
H10	0.820306	-1.584808	1.101154
H11	1.281361	-1.873758	-0.557265

Table S2. Cartesian coordinates for the equilibrium structure of conf. **II** obtained at the B3LYP-D3(BJ)/cc-pVQZ level of theory.

	Cartesian Coordinates (Angstroms) for conf. II		
Atom	X	Y	Z
C1	2.291717	-0.951721	0.000000
C2	2.024395	0.343996	0.000000
C3	0.654953	0.952070	0.000000
N4	-0.391630	-0.038914	0.000000

C5	-1.587352	-0.080417	0.000000
O6	-2.746031	-0.243669	0.000000
H7	3.309926	-1.312178	0.000000
H8	1.499654	-1.687008	0.000000
H9	2.829640	1.069798	0.000000
H10	0.547216	1.597369	-0.876964
H11	0.547216	1.597369	0.876964

Table S3. Cartesian coordinates for the equilibrium structure of conf. **III** obtained at the B3LYP-D3(BJ)/cc-pVQZ level of theory.

	Cartesian Coordinates (Angstroms) for conf. III_a		
Atom	X	Y	Z
C1	2.350828	-0.887879	-0.236582
C2	1.521801	-0.117819	0.451531
C3	0.759177	1.027996	-0.142460
N4	-0.676601	0.884148	0.012132
C5	-1.469818	-0.015149	-0.019987
O6	-2.334358	-0.802568	-0.024026
H7	2.887582	-1.701136	0.230622
H8	2.524595	-0.729798	-1.293434
H9	1.353780	-0.297662	1.507395
H10	0.995818	1.133774	-1.202186
H11	1.037860	1.962365	0.345228
	Cartesian Coordinates (Angstroms) for conf. III_b		
Atom	X	Y	Z
C1	-2.350835	-0.887870	-0.236588
C2	-1.521792	-0.117833	0.451532
C3	-0.759178	1.027999	-0.142441
N4	0.676602	0.884151	0.012119
C5	1.469817	-0.015149	-0.019991
O6	2.334357	-0.802569	-0.024025
H7	-2.887580	-1.701142	0.230600
H8	-2.524623	-0.729753	-1.293431
H9	-1.353749	-0.297712	1.507387
H10	-1.037854	1.962356	0.345274
H11	-0.995840	1.133804	-1.202160

Appendix II: Basis set benchmark using the B3LYP-D3(BJ) method.

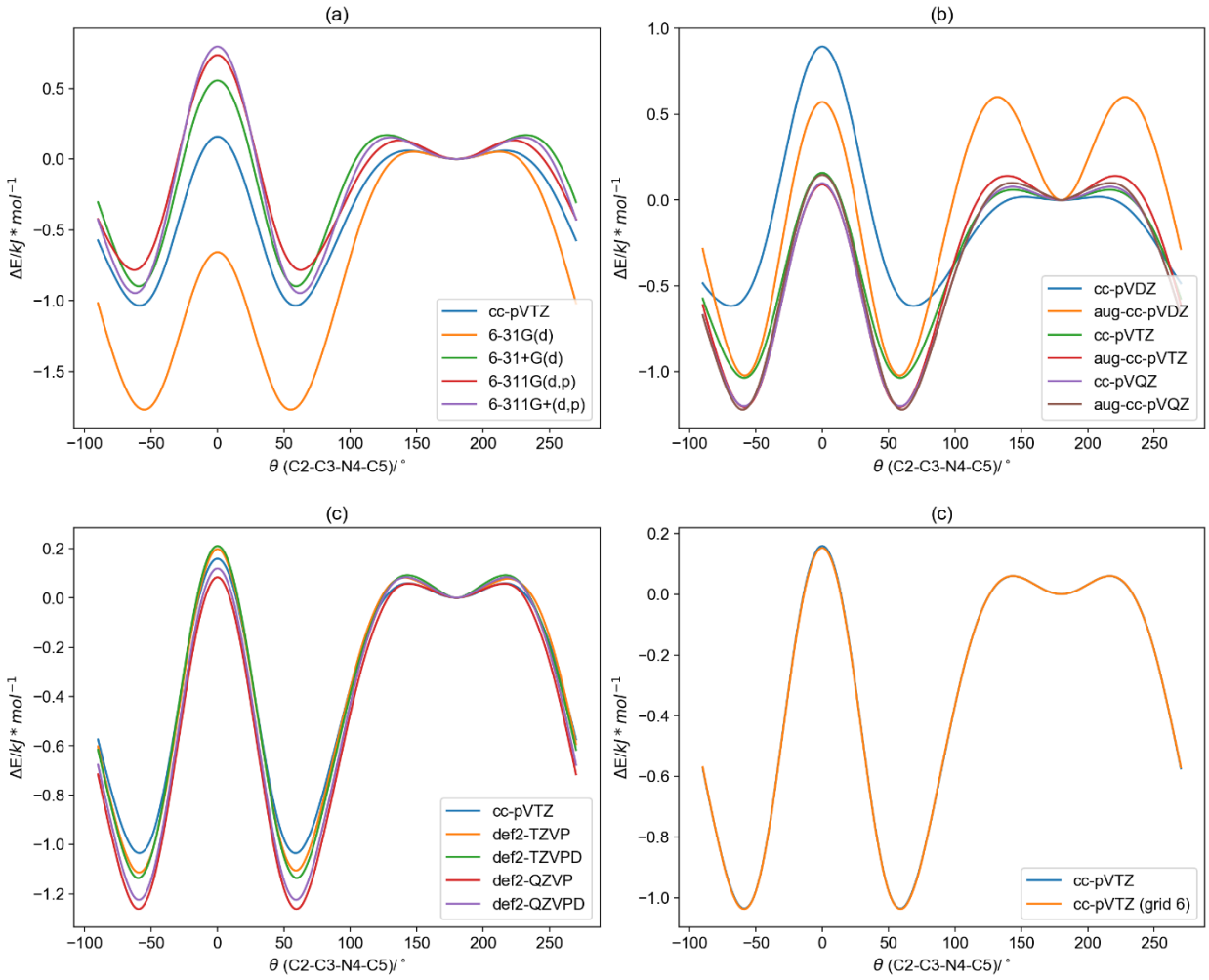

FIG. S1. Potential energy profiles of Route 1 calculated using the B3LYP-D3(BJ) method and different types of basis set: (a). Pople's basis sets, (b). Dunning's basis sets, (c). Karlsruhe's basis sets, (d) integration grid. The default grid 4 was used if not mentioned otherwise.

Appendix III: Measured line lists for conf. **III** and conf. **I**, including their parent and minor isotopologues (^{13}C, ^{15}N and ^{18}O).

Table S4. Assigned transitions for the parent species of conf. **III**.

J''	K_a''	K_c''	F''	J'	K_a'	K_c'	F'	ν_{obs} /MHz	$\nu_{obs - calc}$/MHz
2	1	2	1	1	1	1	0	7360.558	-0.001
2	1	2	1	1	1	1	1	7360.901	-0.002
2	1	2	3	1	1	1	2	7361.030	-0.002
2	1	2	2	1	1	1	1	7361.647	-0.002
2	0	2	1	1	0	1	1	7677.892	-0.001
2	0	2	3	1	0	1	2	7678.830	0.000
2	0	2	2	1	0	1	1	7678.881	0.000
2	0	2	1	1	0	1	0	7679.354	-0.001
2	0	2	2	1	0	1	2	7679.464	-0.002
4	1	3	3	4	0	4	4	7916.846	-0.002
4	1	3	5	4	0	4	4	7916.949	0.000
4	1	3	4	4	0	4	4	7917.346	0.001
4	1	3	5	4	0	4	5	7917.654	0.001
4	1	3	3	4	0	4	3	7917.730	-0.002
4	1	3	4	4	0	4	5	7918.049	0.000
4	1	3	4	4	0	4	3	7918.229	-0.001
1	1	1	1	0	0	0	1	9776.195	0.001
1	1	1	2	0	0	0	1	9776.332	0.000
1	1	1	0	0	0	0	1	9776.539	0.001
4	0	4	3	3	1	3	3	10088.346	0.000
4	0	4	5	3	1	3	4	10089.190	0.000
4	0	4	4	3	1	3	3	10089.230	-0.001
4	0	4	3	3	1	3	2	10089.241	0.001
4	0	4	4	3	1	3	4	10089.891	-0.003
3	1	3	2	2	1	2	2	11032.537	0.000
3	1	3	4	2	1	2	3	11033.248	0.000
3	1	3	2	2	1	2	1	11033.282	0.000
3	1	3	3	2	1	2	2	11033.430	-0.001
3	1	3	3	2	1	2	3	11033.910	0.000
3	0	3	2	2	0	2	2	11483.588	0.000
3	0	3	4	2	0	2	3	11484.458	0.000
3	0	3	3	2	0	2	2	11484.494	0.000
3	0	3	2	2	0	2	1	11484.574	-0.002
3	0	3	3	2	0	2	3	11485.128	-0.001
3	2	1	2	2	2	0	1	11592.752	0.002
3	2	1	4	2	2	0	3	11593.096	0.000

3	2	1	3	2	2	0	2	11593.710	0.001
3	2	1	2	2	2	0	2	11593.738	0.000
3	1	2	2	2	1	1	2	12026.696	-0.001
3	1	2	2	2	1	1	1	12026.924	-0.001
3	1	2	4	2	1	1	3	12026.954	-0.001
3	1	2	3	2	1	1	2	12027.124	-0.001
3	1	2	3	2	1	1	3	12027.272	0.000
2	1	2	1	1	0	1	1	13290.375	-0.001
2	1	2	2	1	0	1	1	13291.120	0.000
2	1	2	3	1	0	1	2	13291.227	0.001
2	1	2	2	1	0	1	2	13291.705	-0.001
2	1	2	1	1	0	1	0	13291.837	-0.001
2	1	1	3	1	0	1	2	14285.497	0.002
2	1	1	2	1	0	1	2	14285.644	0.002
2	1	1	1	1	0	1	0	14286.292	0.001
5	0	5	4	4	1	4	4	14358.564	0.000
5	0	5	5	4	1	4	4	14359.450	0.001
5	0	5	6	4	1	4	5	14359.465	0.003
5	0	5	4	4	1	4	3	14359.504	0.001
5	0	5	5	4	1	4	5	14360.199	0.002
4	1	4	5	3	1	3	4	14695.785	0.004
4	1	4	3	3	1	3	2	14695.824	0.004
4	1	4	4	3	1	3	3	14695.872	0.006
4	0	4	5	3	0	3	4	15250.378	0.002
4	0	4	4	3	0	3	3	15250.410	0.002
4	0	4	3	3	0	3	2	15250.431	0.001
4	3	2	5	3	3	1	4	15412.980	0.000
4	3	2	4	3	3	1	3	15413.556	0.000
4	3	1	5	3	3	0	4	15415.042	-0.001
4	3	1	4	3	3	0	3	15415.618	0.000
4	2	2	3	3	2	1	2	15508.408	0.004
4	2	2	3	3	2	1	3	15508.434	0.001
4	2	2	5	3	2	1	4	15508.473	0.003
4	2	2	4	3	2	1	3	15508.723	0.003
4	1	3	3	3	1	2	3	16018.445	-0.003
4	1	3	5	3	1	2	4	16018.864	-0.003
4	1	3	3	3	1	2	2	16018.876	-0.001
4	1	3	4	3	1	2	3	16018.943	-0.002
4	1	3	4	3	1	2	4	16019.261	-0.003
5	1	5	4	4	1	4	4	18345.332	-0.003
5	1	5	6	4	1	4	5	18346.243	-0.002
5	1	5	4	4	1	4	3	18346.272	-0.003
5	1	5	5	4	1	4	4	18346.294	-0.001

5	1	5	5	4	1	4	5	18347.040	-0.003

Table S5. Assigned transitions for the ^{13}C1 species of conf. **III**.

J”	K_a”	K_c”	F”	J’	K_a’	K_c’	F’	ν_{obs} /MHz	$\nu_{obs - calc}$/MHz
2	0	2	3	1	0	1	2	7513.108	-0.001
2	1	1	3	1	1	0	2	7848.272	0.000
3	1	3	2	2	1	2	2	10797.252	-0.001
3	1	3	4	2	1	2	3	10797.963	0.000
3	1	3	3	2	1	2	2	10798.140	-0.003
3	1	3	3	2	1	2	3	10798.620	-0.002
3	0	3	2	2	0	2	2	11236.547	0.000
3	0	3	4	2	0	2	3	11237.401	0.000
3	0	3	3	2	0	2	2	11237.437	0.000
3	0	3	2	2	0	2	1	11237.513	-0.003
3	0	3	3	2	0	2	3	11238.059	0.000
3	2	1	2	2	2	0	1	11340.819	-0.001
3	2	1	4	2	2	0	3	11341.157	0.000
3	2	1	3	2	2	0	2	11341.758	0.000
3	1	2	2	2	1	1	1	11763.982	0.000
3	1	2	4	2	1	1	3	11764.013	0.001
3	1	2	3	2	1	1	2	11764.180	0.000
4	1	4	5	3	1	3	4	14382.741	0.001
4	1	4	3	3	1	3	2	14382.781	0.002
4	1	4	4	3	1	3	3	14382.827	0.003
4	1	4	4	3	1	3	4	14383.484	0.001
4	0	4	5	3	0	3	4	14923.746	0.001
4	0	4	4	3	0	3	3	14923.778	0.000
4	0	4	3	3	0	3	2	14923.801	0.003
4	2	3	5	3	2	2	4	15042.651	-0.002
4	2	2	3	3	2	1	2	15170.208	0.002
4	2	2	5	3	2	1	4	15170.271	0.000
4	2	2	4	3	2	1	3	15170.516	0.001
4	1	3	5	3	1	2	4	15669.055	-0.004
4	1	3	3	3	1	2	2	15669.069	0.002
4	1	3	4	3	1	2	3	15669.135	-0.001
5	1	5	6	4	1	4	5	17955.957	-0.004

Table S6. Assigned transitions for the ^{13}C2 species of conf. **III**.

J”	K_a”	K_c”	F”	J’	K_a’	K_c’	F’	ν_{obs} /MHz	$\nu_{obs - calc}$/MHz
2	1	2	2	1	1	1	2	7301.672	0.001
2	0	2	3	1	0	1	2	7612.572	-0.001
2	1	1	3	1	1	0	2	7950.079	0.001
3	1	3	4	2	1	2	3	10943.819	-0.001
3	1	3	3	2	1	2	2	10944.000	-0.002
3	0	3	2	2	0	2	2	11385.535	0.000
3	0	3	4	2	0	2	3	11386.401	0.000
3	0	3	3	2	0	2	2	11386.434	-0.003
3	0	3	2	2	0	2	1	11386.517	-0.001
3	0	3	3	2	0	2	3	11387.067	-0.002
3	2	2	2	2	2	1	1	11438.678	-0.001
3	2	2	4	2	2	1	3	11439.022	-0.003
3	2	2	3	2	2	1	2	11439.650	0.000
3	2	1	2	2	2	0	1	11490.420	0.003
3	2	1	4	2	2	0	3	11490.762	0.000
3	2	1	3	2	2	0	2	11491.376	0.003
3	1	2	2	2	1	1	1	11916.647	0.003
3	1	2	4	2	1	1	3	11916.675	0.001
3	1	2	3	2	1	1	2	11916.845	0.001
4	1	4	5	3	1	3	4	14577.129	0.003
4	1	4	3	3	1	3	2	14577.168	0.002
4	1	4	4	3	1	3	3	14577.216	0.005
4	0	4	5	3	0	3	4	15122.048	-0.001
4	0	4	4	3	0	3	3	15122.079	-0.002
4	0	4	3	3	0	3	2	15122.103	0.000
4	2	3	5	3	2	2	4	15241.645	-0.002
4	2	3	4	3	2	2	3	15241.913	-0.001
4	1	3	5	3	1	2	4	15872.509	-0.002
4	1	3	3	3	1	2	2	15872.522	0.001
4	1	3	4	3	1	2	3	15872.589	0.000
5	1	5	6	4	1	4	5	18198.804	-0.002
5	1	5	4	4	1	4	3	18198.833	-0.002
5	1	5	5	4	1	4	4	18198.854	-0.001
5	0	5	6	4	0	4	5	18809.301	0.004
5	0	5	4	4	0	4	3	18809.330	0.001

Table S7. Assigned transitions for the ^{13}C3 species of conf. **III**.

J''	K_a''	K_c''	F''	J'	K_a'	K_c'	F'	ν_{obs} /MHz	$\nu_{obs - calc}$/MHz
2	1	2	3	1	1	1	2	7326.251	-0.001
2	1	2	2	1	1	1	1	7326.870	-0.002
2	0	2	3	1	0	1	2	7648.359	0.001
2	0	2	1	1	0	1	0	7648.887	0.001
2	1	1	3	1	1	0	2	7999.080	0.000
3	1	3	4	2	1	2	3	10980.656	0.002
3	1	3	2	2	1	2	1	10980.685	-0.004
3	1	3	3	2	1	2	2	10980.838	0.000
3	0	3	2	2	0	2	2	11436.122	-0.001
3	0	3	4	2	0	2	3	11436.998	0.000
3	0	3	3	2	0	2	2	11437.035	-0.001
3	0	3	2	2	0	2	1	11437.116	-0.001
3	0	3	3	2	0	2	3	11437.674	-0.001
3	2	2	2	2	2	1	1	11494.214	-0.001
3	2	2	4	2	2	1	3	11494.564	-0.001
3	2	2	3	2	2	1	2	11495.195	0.000
3	2	1	2	2	2	0	1	11550.904	0.002
3	2	1	4	2	2	0	3	11551.251	0.002
3	2	1	3	2	2	0	2	11551.869	0.004
3	1	2	2	2	1	1	1	11989.342	0.004
3	1	2	4	2	1	1	3	11989.369	0.000
3	1	2	3	2	1	1	2	11989.541	0.000
4	1	4	3	3	1	3	3	14624.046	0.000
4	1	4	5	3	1	3	4	14624.910	0.005
4	1	4	3	3	1	3	2	14624.948	0.003
4	1	4	4	3	1	3	4	14625.660	0.002
4	0	4	5	3	0	3	4	15183.940	0.001
4	0	4	4	3	0	3	3	15183.972	-0.001
4	0	4	3	3	0	3	2	15183.991	-0.002
4	1	3	5	3	1	2	4	15967.853	-0.004
4	1	3	3	3	1	2	2	15967.866	0.000
4	1	3	4	3	1	2	3	15967.934	-0.002
5	1	5	6	4	1	4	5	18256.533	-0.004
5	1	5	5	4	1	4	4	18256.583	-0.004
5	0	5	6	4	0	4	5	18878.323	0.004
5	0	5	5	4	0	4	4	18878.352	0.001

Table S8. Assigned transitions for the ^{15}N4 species of conf. **III**.

J''	K_a''	K_c''	J'	K_a'	K_c'	ν_{obs} /MHz	$\nu_{obs - calc}$/MHz
2	1	2	1	1	1	7334.392	-0.001
2	0	2	1	0	1	7655.542	-0.001
2	1	1	1	1	0	8005.151	0.000
3	1	3	2	1	2	10992.825	0.001
3	2	1	2	2	0	11561.263	0.000
3	1	2	2	1	1	11998.459	0.000
4	1	4	3	1	3	14641.255	0.001
4	0	4	3	0	3	15199.358	0.000
4	1	3	3	1	2	15980.134	0.000
5	1	5	4	1	4	18277.187	0.000

Table S9. Assigned transitions for the ^{13}C5 species of conf. **III**.

J''	K_a''	K_c''	F''	J'	K_a'	K_c'	F'	ν_{obs} /MHz	$\nu_{obs - calc}$/MHz
2	1	2	3	1	1	1	2	7305.530	-0.002
2	1	2	2	1	1	1	1	7306.147	-0.002
2	0	2	1	1	0	1	1	7617.680	0.001
2	0	2	3	1	0	1	2	7618.616	0.000
2	0	2	2	1	0	1	1	7618.665	-0.001
2	0	2	1	1	0	1	0	7619.140	0.001
2	0	2	2	1	0	1	2	7619.251	0.001
2	1	1	3	1	1	0	2	7958.003	0.002
2	1	1	2	1	1	0	1	7958.599	0.003
3	1	3	4	2	1	2	3	10950.276	0.001
3	1	3	2	2	1	2	1	10950.310	0.001
3	1	3	3	2	1	2	2	10950.458	0.001
3	1	3	3	2	1	2	3	10950.937	0.001
3	0	3	2	2	0	2	2	11394.384	-0.001
3	0	3	4	2	0	2	3	11395.253	0.000
3	0	3	3	2	0	2	2	11395.290	0.001
3	0	3	2	2	0	2	1	11395.370	-0.001
3	0	3	3	2	0	2	3	11395.923	-0.001
3	2	2	2	2	2	1	1	11447.887	0.001
3	2	2	4	2	2	1	3	11448.234	0.000
3	2	2	3	2	2	1	2	11448.860	0.000
3	2	1	2	2	2	0	1	11499.966	0.002
3	2	1	4	2	2	0	3	11500.311	0.002
3	2	1	3	2	2	0	2	11500.925	0.003
3	1	2	2	2	1	1	2	11928.246	0.000

3	1	2	2	2	1	1	1	11928.475	0.001
3	1	2	4	2	1	1	3	11928.504	0.000
3	1	2	3	2	1	1	2	11928.675	0.001
4	0	4	5	3	0	3	4	15133.464	0.000
4	0	4	4	3	0	3	3	15133.496	0.000
4	0	4	3	3	0	3	2	15133.518	0.000
4	2	3	3	3	2	2	2	15253.789	0.000
4	2	3	5	3	2	2	4	15253.856	-0.001
4	1	3	5	3	1	2	4	15888.174	-0.004
4	1	3	3	3	1	2	2	15888.186	-0.001
4	1	3	4	3	1	2	3	15888.252	-0.004
5	1	5	6	4	1	4	5	18209.300	-0.003
5	1	5	5	4	1	4	4	18209.350	-0.003
5	0	5	6	4	0	4	5	18822.969	0.002
5	0	5	5	4	0	4	4	18823.000	0.002

Table S10. Assigned transitions for the ^{18}O6 species of conf. **III**.

J”	K_a”	K_c”	F”	J’	K_a’	K_c’	F’	ν_{obs} /MHz	$\nu_{obs - calc}$/MHz
2	1	2	3	1	1	1	2	7070.243	-0.002
2	0	2	3	1	0	1	2	7371.822	0.000
2	1	1	1	1	1	0	0	7697.366	0.000
2	1	1	3	1	1	0	2	7698.131	0.000
3	1	3	4	2	1	2	3	10597.828	0.001
3	1	3	2	2	1	2	1	10597.860	0.001
3	1	3	3	2	1	2	2	10598.014	0.000
3	0	3	4	2	0	2	3	11027.000	0.001
3	0	3	3	2	0	2	2	11027.033	-0.002
3	0	3	2	2	0	2	1	11027.120	0.000
5	1	5	6	4	1	4	5	17624.267	0.000
5	1	5	4	4	1	4	3	17624.296	-0.001
5	1	5	5	4	1	4	4	17624.319	0.001
5	0	5	6	4	0	4	5	18219.005	-0.001
5	0	5	5	4	0	4	4	18219.037	0.002
5	0	5	4	4	0	4	3	18219.037	-0.001

Table S11. Assigned transitions for the parent species of conf. **I**.

J”	K_a”	K_c”	V"	F”	J’	K_a’	K_c’	V'	F”	ν_{obs} /MHz	$\nu_{obs - calc}$/MHz
1	1	0	0	2	1	0	1	0	1	5485.253	0.001

1	1	0	0	1	1	0	1	0	2	5485.451	0.002
1	1	0	0	2	1	0	1	0	2	5485.847	0.001
1	1	0	0	1	1	0	1	0	0	5486.342	0.001
1	1	0	1	1	1	0	1	1	1	5486.563	0.000
1	1	0	1	2	1	0	1	1	1	5486.960	0.000
1	1	0	1	1	1	0	1	1	2	5487.156	-0.001
1	1	0	1	2	1	0	1	1	2	5487.555	0.001
2	1	1	0	2	2	0	2	0	2	6064.537	-0.001
2	1	1	0	3	2	0	2	0	3	6064.973	0.001
2	1	1	0	1	2	0	2	0	1	6065.215	0.002
2	1	1	1	2	2	0	2	1	2	6065.629	-0.001
2	1	1	1	3	2	0	2	1	3	6066.062	-0.002
2	1	1	1	1	2	0	2	1	1	6066.304	-0.002
2	1	2	1	1	2	0	2	0	2	6391.574	-0.003
2	1	2	1	3	2	0	2	0	2	6391.809	-0.003
2	1	2	1	2	2	0	2	0	2	6392.239	0.001
2	1	2	1	3	2	0	2	0	3	6392.457	-0.001
2	1	2	1	2	2	0	2	0	3	6392.883	0.000
2	1	2	1	2	2	0	2	0	1	6393.243	0.001
1	1	1	1	1	1	0	1	0	1	6888.778	0.002
1	1	1	1	2	1	0	1	0	1	6888.974	0.001
1	1	1	1	0	1	0	1	0	1	6889.270	0.001
1	1	1	1	1	1	0	1	0	2	6889.373	0.002
1	1	1	1	2	1	0	1	0	2	6889.569	0.001
1	1	1	1	1	1	0	1	0	0	6890.265	0.002
3	1	2	1	3	3	0	3	1	3	7008.108	0.000
3	1	2	1	4	3	0	3	1	4	7008.403	0.000
3	1	2	1	2	3	0	3	1	2	7008.506	-0.001
3	1	2	0	3	3	0	3	0	3	7010.285	0.001
3	1	2	0	4	3	0	3	0	4	7010.578	-0.001
3	1	2	0	2	3	0	3	0	2	7010.681	-0.001
1	1	0	0	1	0	0	0	1	1	7893.785	-0.001
1	1	0	0	2	0	0	0	1	1	7894.183	0.000
1	1	0	0	0	0	0	0	1	1	7894.777	-0.001
2	1	2	1	1	1	1	1	1	0	8158.137	-0.002
2	1	2	1	3	1	1	1	1	2	8158.670	-0.001
2	1	2	0	1	1	1	1	0	0	8159.026	0.000
2	1	2	1	2	1	1	1	1	1	8159.293	0.000
2	1	2	0	3	1	1	1	0	2	8159.559	0.001
2	1	2	0	2	1	1	1	0	1	8160.180	-0.001
4	1	3	1	4	4	0	4	1	4	8392.019	0.001
4	1	3	1	5	4	0	4	1	5	8392.264	0.000
4	1	3	1	3	4	0	4	1	3	8392.328	0.001

4	1	3	0	4	4	0	4	0	4	8397.448	-0.002
4	1	3	0	5	4	0	4	0	5	8397.692	-0.003
4	1	3	0	3	4	0	4	0	3	8397.756	-0.003
3	0	3	1	2	2	1	2	1	2	8421.451	-0.003
3	0	3	1	4	2	1	2	1	3	8422.117	-0.001
3	0	3	1	3	2	1	2	1	2	8422.371	-0.003
3	0	3	1	3	2	1	2	1	3	8422.798	-0.002
3	0	3	0	2	2	1	2	0	2	8429.045	0.002
3	0	3	0	4	2	1	2	0	3	8429.709	0.001
3	0	3	0	3	2	1	2	0	2	8429.966	0.002
3	0	3	0	3	2	1	2	0	3	8430.391	0.002
2	0	2	1	1	1	0	1	1	1	8652.366	0.001
2	0	2	1	3	1	0	1	1	2	8653.316	-0.001
2	0	2	1	1	1	0	1	1	0	8653.848	-0.002
2	0	2	1	2	1	0	1	1	2	8653.961	-0.001
2	0	2	0	1	1	0	1	0	1	8654.829	0.001
2	0	2	0	3	1	0	1	0	2	8655.782	0.001
2	0	2	0	1	1	0	1	0	0	8656.315	0.001
2	0	2	0	2	1	0	1	0	2	8656.428	0.002
2	1	1	1	1	1	1	0	1	0	9231.112	-0.002
2	1	1	1	3	1	1	0	1	2	9231.826	-0.001
2	1	1	1	2	1	1	0	1	1	9232.434	-0.001
2	1	1	0	1	1	1	0	0	0	9234.195	0.002
2	1	1	0	3	1	1	0	0	2	9234.908	0.002
2	1	1	0	2	1	1	0	0	1	9235.515	0.000
1	1	1	0	1	0	0	0	0	1	9296.227	0.002
1	1	1	0	2	0	0	0	0	1	9296.424	0.002
1	1	1	0	0	0	0	0	0	1	9296.720	0.002
1	1	1	1	1	0	0	0	1	1	9297.708	0.000
1	1	1	1	2	0	0	0	1	1	9297.905	0.000
1	1	1	1	0	0	0	0	1	1	9298.201	0.000
1	1	0	1	1	0	0	0	0	1	11774.742	0.002
1	1	0	1	2	0	0	0	0	1	11775.140	0.003
1	1	0	1	0	0	0	0	0	1	11775.735	0.001
3	1	3	1	2	2	1	2	1	2	12210.327	-0.001
3	1	3	1	4	2	1	2	1	3	12210.968	0.002
3	1	3	1	3	2	1	2	1	2	12211.147	-0.003
3	1	3	1	3	2	1	2	1	3	12211.575	0.000
3	1	3	0	2	2	1	2	0	2	12213.583	0.000
3	1	3	0	4	2	1	2	0	3	12214.222	0.000
3	1	3	0	3	2	1	2	0	2	12214.405	-0.001
3	1	3	0	3	2	1	2	0	3	12214.831	0.000
2	1	1	0	1	1	0	1	1	1	12781.094	0.003

2	1	1	0	2	1	0	1	1	1	12781.422	0.001
2	1	1	0	3	1	0	1	1	2	12781.804	0.001
2	1	1	0	2	1	0	1	1	2	12782.012	-0.003
2	1	1	0	1	1	0	1	1	0	12782.578	0.002
3	0	3	1	2	2	0	2	1	2	12877.206	0.000
3	0	3	1	4	2	0	2	1	3	12878.089	-0.001
3	0	3	1	3	2	0	2	1	2	12878.126	-0.001
3	0	3	1	3	2	0	2	1	3	12878.770	-0.002
3	0	3	0	2	2	0	2	0	2	12880.391	0.001
3	0	3	0	4	2	0	2	0	3	12881.275	0.001
3	0	3	0	3	2	0	2	0	2	12881.312	0.001
3	0	3	0	3	2	0	2	0	3	12881.957	0.001
3	2	2	1	2	2	2	1	1	1	13042.447	0.000
3	2	2	1	4	2	2	1	1	3	13042.802	0.001
3	2	2	1	3	2	2	1	1	2	13043.438	0.000
3	2	2	0	2	2	2	1	0	1	13046.291	0.000
3	2	2	0	4	2	2	1	0	3	13046.647	0.002
3	2	2	0	3	2	2	1	0	2	13047.283	0.001
2	1	2	0	1	1	0	1	0	1	13106.516	0.000
2	1	2	0	2	1	0	1	0	1	13107.179	0.000
2	1	2	0	3	1	0	1	0	2	13107.347	0.000
2	1	2	0	2	1	0	1	0	2	13107.773	0.001
2	1	2	0	1	1	0	1	0	0	13108.003	0.001
2	1	2	1	1	1	0	1	1	1	13108.458	-0.001
2	1	2	1	3	1	0	1	1	2	13109.288	-0.001
2	1	2	1	2	1	0	1	1	2	13109.716	0.001
2	1	2	1	1	1	0	1	1	0	13109.941	-0.003
4	0	4	1	5	3	1	3	1	4	13200.557	-0.002
4	0	4	1	4	3	1	3	1	3	13200.663	-0.001
3	2	1	1	2	2	2	0	1	1	13206.065	0.000
3	2	1	1	4	2	2	0	1	3	13206.418	0.002
3	2	1	1	3	2	2	0	1	2	13207.039	0.000
4	0	4	0	5	3	1	3	0	4	13208.344	0.003
4	0	4	0	4	3	1	3	0	3	13208.449	0.003
3	2	1	0	2	2	2	0	0	1	13210.610	-0.001
3	2	1	0	4	2	2	0	0	3	13210.962	0.001
3	2	1	0	3	2	2	0	0	2	13211.585	0.000
3	1	2	1	2	2	1	1	1	2	13820.082	0.000
3	1	2	1	4	2	1	1	1	3	13820.429	0.000
3	1	2	1	3	2	1	1	1	2	13820.605	0.000
3	1	2	0	4	2	1	1	0	3	13826.880	0.000
3	1	2	0	3	2	1	1	0	2	13827.060	0.004
3	2	1	0	3	3	1	2	0	3	14267.534	-0.003

3	2	1	0	4	3	1	2	0	4	14267.944	-0.002
3	2	1	0	2	3	1	2	0	2	14268.088	-0.001
3	2	1	1	3	3	1	2	1	3	14276.982	0.001
3	2	1	1	4	3	1	2	1	4	14277.391	0.001
3	2	1	1	2	3	1	2	1	2	14277.533	0.001
2	2	0	0	2	2	1	1	0	2	14883.009	0.001
2	2	0	1	2	2	1	1	1	2	14890.547	0.001
2	2	0	1	3	2	1	1	1	3	14891.403	0.001
2	2	0	1	1	2	1	1	1	1	14891.879	0.001
4	1	4	1	3	3	1	3	1	3	16237.969	0.002
4	1	4	1	5	3	1	3	1	4	16238.755	0.001
4	1	4	1	3	3	1	3	1	2	16238.788	-0.001
4	1	4	1	4	3	1	3	1	3	16238.840	0.000
4	1	4	1	4	3	1	3	1	4	16239.448	-0.001
4	1	4	0	3	3	1	3	0	3	16240.539	0.000
4	1	4	0	5	3	1	3	0	4	16241.328	0.001
4	1	4	0	3	3	1	3	0	2	16241.360	-0.001
4	1	4	0	4	3	1	3	0	3	16241.412	0.000
4	1	4	0	4	3	1	3	0	4	16242.021	0.000
2	2	1	0	2	2	1	2	0	2	16454.711	0.001
2	2	1	0	3	2	1	2	0	2	16455.349	0.003
2	2	1	0	2	2	1	2	0	1	16455.373	0.001
2	2	1	0	3	2	1	2	0	3	16455.771	-0.001
2	2	1	0	1	2	1	2	0	1	16456.363	0.001
2	2	1	1	2	2	1	2	1	2	16459.110	-0.003
2	2	1	1	2	2	1	2	1	1	16459.774	-0.001
2	2	1	1	3	2	1	2	1	3	16460.173	-0.003
2	2	1	1	1	2	1	2	1	1	16460.766	0.000
2	1	1	1	1	1	0	1	0	1	16657.619	-0.001
2	1	1	1	2	1	0	1	0	1	16657.945	-0.003
2	1	1	1	3	1	0	1	0	2	16658.330	-0.001
2	1	1	1	2	1	0	1	0	2	16658.540	-0.002
2	1	1	1	1	1	0	1	0	0	16659.104	-0.001
3	1	3	0	2	2	0	2	0	2	16664.928	-0.002
3	1	3	0	3	2	0	2	0	2	16665.751	-0.001
3	1	3	0	4	2	0	2	0	3	16665.786	-0.002
3	1	3	0	2	2	0	2	0	1	16665.932	-0.001
3	1	3	1	3	2	0	2	1	2	16666.902	0.000
3	1	3	1	4	2	0	2	1	3	16666.938	-0.001
3	1	3	1	2	2	0	2	1	1	16667.083	0.000
3	1	3	1	3	2	0	2	1	3	16667.547	0.000
4	0	4	1	3	3	0	3	1	3	16988.542	0.000
4	0	4	1	5	3	0	3	1	4	16989.407	0.000

4	0	4	1	4	3	0	3	1	3	16989.438	-0.001
4	0	4	1	3	3	0	3	1	2	16989.462	0.000
4	0	4	1	4	3	0	3	1	4	16990.120	-0.001
4	0	4	0	3	3	0	3	0	3	16991.990	0.000
4	0	4	0	5	3	0	3	0	4	16992.857	0.001
4	0	4	0	3	3	0	3	0	2	16992.912	0.001
4	0	4	0	4	3	0	3	0	4	16993.570	0.000
3	2	2	0	3	3	1	3	0	3	17287.588	0.002
3	2	2	0	4	3	1	3	0	4	17288.196	0.001
3	2	2	0	2	3	1	3	0	2	17288.410	0.002
3	2	2	1	3	3	1	3	1	3	17291.402	0.001
3	2	2	1	4	3	1	3	1	4	17292.008	-0.002
3	2	2	1	2	3	1	3	1	2	17292.221	-0.002
4	2	3	1	3	3	2	2	1	2	17357.734	0.001
4	2	3	1	5	3	2	2	1	4	17357.803	0.000
4	2	3	1	4	3	2	2	1	3	17358.075	0.000
4	2	3	0	3	3	2	2	0	2	17362.624	0.000
4	2	3	0	5	3	2	2	0	4	17362.694	0.000
4	2	3	0	4	3	2	2	0	3	17362.966	0.000
4	3	2	1	3	3	3	1	1	2	17467.925	0.003
4	3	2	1	5	3	3	1	1	4	17468.153	0.005
4	3	2	1	4	3	3	1	1	3	17468.738	0.004
4	3	2	0	3	3	3	1	0	2	17473.368	-0.004
4	3	2	0	5	3	3	1	0	4	17473.596	-0.002
4	3	2	0	4	3	3	1	0	3	17474.181	-0.003
4	3	1	1	3	3	3	0	1	2	17479.826	0.003
4	3	1	1	5	3	3	0	1	4	17480.054	0.004
4	3	1	1	4	3	3	0	1	3	17480.638	0.004
4	3	1	0	3	3	3	0	0	2	17485.347	-0.005
4	3	1	0	5	3	3	0	0	4	17485.575	-0.004
4	3	1	0	4	3	3	0	0	3	17486.159	-0.004
4	2	2	1	3	3	2	1	1	2	17756.534	0.002
4	2	2	1	5	3	2	1	1	4	17756.603	0.004
4	2	2	1	4	3	2	1	1	3	17756.858	0.003
4	2	2	0	3	3	2	1	0	2	17763.082	-0.004
4	2	2	0	5	3	2	1	0	4	17763.153	0.000
4	2	2	0	4	3	2	1	0	3	17763.408	-0.001
5	0	5	1	6	4	1	4	1	5	17935.623	-0.003
5	0	5	1	5	4	1	4	1	4	17935.673	-0.003
5	0	5	0	6	4	1	4	0	5	17944.176	0.002
5	0	5	0	5	4	1	4	0	4	17944.226	0.001
4	1	3	1	3	3	1	2	1	3	18372.763	0.002
4	1	3	1	5	3	1	2	1	4	18373.271	0.002

4	1	3	1	4	3	1	2	1	3	18373.350	0.001
4	1	3	1	4	3	1	2	1	4	18373.738	0.001
4	1	3	0	3	3	1	2	0	3	18379.462	-0.003
4	1	3	0	5	3	1	2	0	4	18379.972	0.000
4	1	3	0	4	3	1	2	0	3	18380.052	-0.002
4	1	3	0	4	3	1	2	0	4	18380.441	0.000

*Note that, label 'V' represents the tunneling state, 0 for 0^+ and 1 for 0^- state.

Table S12. Assigned transitions for the ^{13}C1 species of conf. **I**.

J"	K_a"	K_c"	V"	F"	J'	K_a'	K_c'	V'	F"	ν_{obs} /MHz	$\nu_{obs - calc}$/MHz
1	1	0	0	2	1	0	1	0	2	5334.535	-0.002
1	1	0	1	2	1	0	1	1	2	5336.213	-0.002
2	1	1	0	2	2	0	2	0	2	5915.690	-0.002
2	1	1	0	3	2	0	2	0	3	5916.127	0.001
2	1	1	0	1	2	0	2	0	1	5916.367	0.000
2	1	1	1	2	2	0	2	1	2	5916.811	-0.001
2	1	1	1	3	2	0	2	1	3	5917.247	0.000
2	1	1	1	1	2	0	2	1	1	5917.486	-0.002
3	1	2	1	3	3	0	3	1	3	6865.465	0.000
3	1	2	1	4	3	0	3	1	4	6865.770	0.003
3	1	2	1	2	3	0	3	1	2	6865.872	-0.001
3	1	2	0	3	3	0	3	0	3	6867.590	0.000
3	1	2	0	4	3	0	3	0	4	6867.894	0.003
3	1	2	0	2	3	0	3	0	2	6867.997	0.000
2	0	2	1	1	1	0	1	1	1	8539.280	0.001
2	0	2	1	3	1	0	1	1	2	8540.207	-0.001
2	0	2	1	1	1	0	1	1	0	8540.726	0.000
2	0	2	1	2	1	0	1	1	2	8540.835	-0.002
2	0	2	0	1	1	0	1	0	1	8541.711	0.002
2	0	2	0	3	1	0	1	0	2	8542.639	0.001
2	0	2	0	1	1	0	1	0	0	8543.160	0.003
2	0	2	0	2	1	0	1	0	2	8543.270	0.001
1	1	1	0	1	0	0	0	0	1	9087.971	0.000
1	1	1	0	2	0	0	0	0	1	9088.155	0.002
1	1	1	0	0	0	0	0	0	1	9088.427	0.001
1	1	1	1	1	0	0	0	1	1	9089.417	-0.001
1	1	1	1	2	0	0	0	1	1	9089.600	0.000
1	1	1	1	0	0	0	0	1	1	9089.872	-0.001
2	1	1	1	1	1	1	0	1	0	9120.533	-0.002
2	1	1	1	3	1	1	0	1	2	9121.239	0.000
2	1	1	1	2	1	1	0	1	1	9121.830	-0.001

2	1	1	0	1	1	1	0	0	0	9123.526	0.003
2	1	1	0	3	1	1	0	0	2	9124.229	0.002
2	1	1	0	2	1	1	0	0	1	9124.819	-0.001
1	1	0	1	2	0	0	0	0	1	11529.332	0.001
3	1	3	1	4	2	1	2	1	3	12040.931	0.001
3	1	3	1	3	2	1	2	1	2	12041.107	-0.003
3	1	3	0	4	2	1	2	0	3	12044.166	0.000
3	1	3	0	3	2	1	2	0	2	12044.346	0.000
2	1	1	0	2	1	0	1	1	1	12558.035	-0.001
2	1	1	0	3	1	0	1	1	2	12558.421	0.001
2	1	1	0	1	1	0	1	1	0	12559.180	0.001
3	0	3	1	2	2	0	2	1	2	12704.195	0.001
3	0	3	1	4	2	0	2	1	3	12705.058	0.000
3	0	3	1	3	2	0	2	1	2	12705.092	-0.004
3	0	3	1	2	2	0	2	1	1	12705.173	-0.001
3	0	3	1	3	2	0	2	1	3	12705.725	-0.001
3	0	3	0	2	2	0	2	0	2	12707.323	0.000
3	0	3	0	4	2	0	2	0	3	12708.188	0.001
3	0	3	0	3	2	0	2	0	2	12708.223	-0.001
3	0	3	0	2	2	0	2	0	1	12708.304	0.001
3	0	3	0	3	2	0	2	0	3	12708.856	0.001
2	1	2	0	1	1	0	1	0	1	12841.304	0.001
2	1	2	0	2	1	0	1	0	1	12841.966	0.001
2	1	2	0	3	1	0	1	0	2	12842.121	0.001
2	1	2	0	2	1	0	1	0	2	12842.545	0.000
2	1	2	1	1	1	0	1	1	1	12843.249	-0.001
2	1	2	1	2	1	0	1	1	1	12843.913	0.003
2	1	2	1	3	1	0	1	1	2	12844.065	0.000
2	1	2	1	2	1	0	1	1	2	12844.492	0.003
3	1	2	1	2	2	1	1	1	1	13653.554	-0.004
3	1	2	1	4	2	1	1	1	3	13653.579	0.000
3	1	2	1	3	2	1	1	1	2	13653.750	0.000
3	1	2	0	2	2	1	1	0	1	13659.925	-0.007
3	1	2	0	4	2	1	1	0	3	13659.951	0.000
3	1	2	0	3	2	1	1	0	2	13660.126	0.003
4	1	4	1	5	3	1	3	1	4	16010.659	0.000
4	1	4	1	3	3	1	3	1	2	16010.695	0.002
4	1	4	1	4	3	1	3	1	3	16010.742	0.000
4	1	4	0	5	3	1	3	0	4	16013.227	0.000
4	1	4	0	3	3	1	3	0	2	16013.264	0.003
4	1	4	0	4	3	1	3	0	3	16013.310	0.000
3	1	3	0	3	2	0	2	0	2	16343.616	-0.006
3	1	3	0	4	2	0	2	0	3	16343.648	0.001

3	1	3	0	2	2	0	2	0	1	16343.783	-0.001
3	1	3	1	3	2	0	2	1	2	16344.759	-0.003
3	1	3	1	4	2	0	2	1	3	16344.789	0.002
3	1	3	1	2	2	0	2	1	1	16344.927	0.001
4	0	4	1	5	3	0	3	1	4	16753.264	0.000
4	0	4	1	4	3	0	3	1	3	16753.297	-0.002
4	0	4	1	3	3	0	3	1	2	16753.318	0.001
4	0	4	0	5	3	0	3	0	4	16756.635	0.000
4	0	4	0	4	3	0	3	0	3	16756.667	-0.001
4	0	4	0	3	3	0	3	0	2	16756.689	0.001
4	1	3	1	5	3	1	2	1	4	18148.816	0.002
4	1	3	1	3	3	1	2	1	2	18148.832	0.004
4	1	3	1	4	3	1	2	1	3	18148.895	0.001
4	1	3	0	5	3	1	2	0	4	18155.433	-0.002
4	1	3	0	3	3	1	2	0	2	18155.449	0.001
4	1	3	0	4	3	1	2	0	3	18155.511	-0.003

*Note that, label ‘V’ represents the tunneling state, 0 for 0^+ and 1 for 0^- state.

Table S13. Assigned transitions for the ^{13}C2 species of conf. **I**.

J”	K_a”	K_c”	V''	F”	J’	K_a’	K_c’	V'	F”	ν_{obs} /MHz	$\nu_{obs - calc}$/MHz
1	1	0	0	2	1	0	1	0	2	5505.693	-0.001
1	1	0	1	2	1	0	1	1	2	5507.352	0.000
2	1	1	0	3	2	0	2	0	3	6066.846	0.001
2	1	1	0	1	2	0	2	0	1	6067.087	0.001
2	1	1	1	2	2	0	2	1	2	6067.509	0.001
2	1	1	1	3	2	0	2	1	3	6067.939	-0.002
2	1	1	1	1	2	0	2	1	1	6068.180	-0.002
3	1	2	1	3	3	0	3	1	3	6978.688	0.000
3	1	2	1	4	3	0	3	1	4	6978.984	0.001
3	1	2	1	2	3	0	3	1	2	6979.086	-0.001
3	1	2	0	3	3	0	3	0	3	6980.700	0.001
3	1	2	0	4	3	0	3	0	4	6980.995	0.001
3	1	2	0	2	3	0	3	0	2	6981.095	-0.002
2	0	2	1	1	1	0	1	1	1	8530.532	0.003
2	0	2	1	3	1	0	1	1	2	8531.479	-0.001
2	0	2	1	1	1	0	1	1	0	8532.012	0.000
2	0	2	1	2	1	0	1	1	2	8532.122	-0.002
2	0	2	0	1	1	0	1	0	1	8532.873	0.003
2	0	2	0	3	1	0	1	0	2	8533.822	0.001
2	0	2	0	1	1	0	1	0	0	8534.356	0.003
2	0	2	0	2	1	0	1	0	2	8534.466	0.001

2	1	1	1	1	1	1	0	1	0	9091.357	-0.001
2	1	1	1	3	1	1	0	1	2	9092.069	-0.001
2	1	1	1	2	1	1	0	1	1	9092.677	-0.001
2	1	1	0	1	1	1	0	0	0	9094.263	0.002
2	1	1	0	3	1	1	0	0	2	9094.973	0.001
2	1	1	0	2	1	1	0	0	1	9095.580	0.000
1	1	1	0	1	0	0	0	0	1	9269.255	0.000
1	1	1	0	2	0	0	0	0	1	9269.455	0.003
1	1	1	0	0	0	0	0	0	1	9269.748	0.001
1	1	1	1	1	0	0	0	1	1	9270.693	-0.001
1	1	1	1	2	0	0	0	1	1	9270.890	-0.001
1	1	1	1	0	0	0	0	1	1	9271.184	-0.002
1	1	0	1	2	0	0	0	0	1	11683.053	0.001
3	1	3	1	4	2	1	2	1	3	12048.963	0.001
3	1	3	1	3	2	1	2	1	2	12049.143	-0.003
3	1	3	0	4	2	1	2	0	3	12052.096	0.001
3	1	3	0	3	2	1	2	0	2	12052.279	0.001
3	0	3	1	2	2	0	2	1	2	12700.578	-0.001
3	0	3	1	4	2	0	2	1	3	12701.461	0.000
3	0	3	1	3	2	0	2	1	2	12701.495	-0.003
3	0	3	1	2	2	0	2	1	1	12701.580	-0.001
3	0	3	1	3	2	0	2	1	3	12702.141	-0.001
3	0	3	0	2	2	0	2	0	2	12703.626	-0.001
3	0	3	0	4	2	0	2	0	3	12704.510	0.001
3	0	3	0	3	2	0	2	0	2	12704.544	-0.002
3	0	3	0	2	2	0	2	0	1	12704.630	0.001
3	0	3	0	3	2	0	2	0	3	12705.192	0.003
2	1	1	0	2	1	0	1	1	1	12710.960	-0.001
2	1	1	0	3	1	0	1	1	2	12711.345	0.002
2	1	1	0	1	1	0	1	1	0	12712.117	0.000
2	1	2	0	1	1	0	1	0	1	13032.704	-0.003
2	1	2	0	2	1	0	1	0	1	13033.368	-0.001
2	1	2	0	3	1	0	1	0	2	13033.537	0.000
2	1	2	0	2	1	0	1	0	2	13033.965	0.003
2	1	2	1	1	1	0	1	1	1	13034.586	0.000
2	1	2	1	2	1	0	1	1	1	13035.249	0.002
2	1	2	1	3	1	0	1	1	2	13035.415	0.000
2	1	2	1	2	1	0	1	1	2	13035.842	0.002
3	1	2	1	2	2	1	1	1	1	13612.480	-0.005
3	1	2	1	4	2	1	1	1	3	13612.504	0.001
3	1	2	1	3	2	1	1	1	2	13612.679	0.000
3	1	2	0	2	2	1	1	0	1	13618.632	-0.007
3	1	2	0	4	2	1	1	0	3	13618.658	0.001

3	1	2	0	3	2	1	1	0	2	13618.836	0.004
4	1	4	1	5	3	1	3	1	4	16025.276	0.001
4	1	4	1	3	3	1	3	1	2	16025.313	0.003
4	1	4	1	4	3	1	3	1	3	16025.359	-0.001
4	1	4	0	5	3	1	3	0	4	16027.731	0.000
4	1	4	0	3	3	1	3	0	2	16027.768	0.002
4	1	4	0	4	3	1	3	0	3	16027.816	0.000
3	1	3	0	3	2	0	2	0	2	16551.772	-0.003
3	1	3	0	4	2	0	2	0	3	16551.811	0.000
3	1	3	0	2	2	0	2	0	1	16551.954	-0.002
3	1	3	1	3	2	0	2	1	2	16552.860	-0.001
3	1	3	1	4	2	0	2	1	3	16552.898	0.001
3	1	3	1	2	2	0	2	1	1	16553.042	0.001
4	0	4	1	5	3	0	3	1	4	16764.297	0.000
4	0	4	1	4	3	0	3	1	3	16764.328	-0.001
4	0	4	1	3	3	0	3	1	2	16764.350	-0.002
4	0	4	0	5	3	0	3	0	4	16767.629	0.000
4	0	4	0	4	3	0	3	0	3	16767.660	-0.001
4	0	4	0	3	3	0	3	0	2	16767.684	0.000
4	1	3	1	5	3	1	2	1	4	18099.486	0.002
4	1	3	1	3	3	1	2	1	2	18099.503	0.005
4	1	3	1	4	3	1	2	1	3	18099.566	0.001
4	1	3	0	5	3	1	2	0	4	18105.851	-0.002
4	1	3	0	3	3	1	2	0	2	18105.869	0.001
4	1	3	0	4	3	1	2	0	3	18105.930	-0.004

*Note that, label ‘V’ represents the tunneling state, 0 for 0^+ and 1 for 0^- state.

Table S14. Assigned transitions for the ^{13}C3 species of conf. **I**.

J”	K_a”	K_c”	V"	F”	J’	K_a’	K_c’	V'	F”	ν_{obs} /MHz	$\nu_{obs - calc}$/MHz
1	1	0	0	2	1	0	1	0	2	5368.122	-0.001
1	1	0	1	2	1	0	1	1	2	5369.749	-0.001
2	1	1	0	2	2	0	2	0	2	5953.478	-0.002
2	1	1	0	3	2	0	2	0	3	5953.914	0.001
2	1	1	0	1	2	0	2	0	1	5954.155	0.001
2	1	1	1	2	2	0	2	1	2	5954.699	0.000
2	1	1	1	3	2	0	2	1	3	5955.133	0.000
2	1	1	1	1	2	0	2	1	1	5955.373	-0.001
3	1	2	1	3	3	0	3	1	3	6910.572	0.001
3	1	2	1	4	3	0	3	1	4	6910.864	0.000
3	1	2	1	2	3	0	3	1	2	6910.966	-0.001
3	1	2	0	3	3	0	3	0	3	6912.803	0.000

3	1	2	0	4	3	0	3	0	4	6913.095	-0.001
3	1	2	0	2	3	0	3	0	2	6913.197	0.000
2	0	2	1	1	1	0	1	1	1	8603.751	0.000
2	0	2	1	3	1	0	1	1	2	8604.714	-0.001
2	0	2	1	1	1	0	1	1	0	8605.253	-0.001
2	0	2	1	2	1	0	1	1	2	8605.365	-0.002
2	0	2	0	1	1	0	1	0	1	8606.131	0.002
2	0	2	0	3	1	0	1	0	2	8607.095	0.001
2	0	2	0	1	1	0	1	0	0	8607.635	0.001
2	0	2	0	2	1	0	1	0	2	8607.748	0.001
1	1	1	0	1	0	0	0	0	1	9149.961	0.000
1	1	1	0	2	0	0	0	0	1	9150.166	0.000
1	1	1	0	0	0	0	0	0	1	9150.473	0.001
1	1	1	1	1	0	0	0	1	1	9151.377	-0.001
1	1	1	1	2	0	0	0	1	1	9151.581	0.000
1	1	1	1	0	0	0	0	1	1	9151.888	0.000
2	1	1	1	1	1	1	0	1	0	9189.379	-0.002
2	1	1	1	3	1	1	0	1	2	9190.097	-0.001
2	1	1	1	2	1	1	0	1	1	9190.714	-0.001
2	1	1	0	1	1	1	0	0	0	9192.169	0.002
2	1	1	0	3	1	1	0	0	2	9192.886	0.001
2	1	1	0	2	1	1	0	0	1	9193.500	-0.001
1	1	0	1	2	0	0	0	0	1	11604.716	0.003
3	1	3	1	4	2	1	2	1	3	12131.781	0.001
3	1	3	1	3	2	1	2	1	2	12131.963	-0.003
3	1	3	0	4	2	1	2	0	3	12135.170	0.000
3	1	3	0	3	2	1	2	0	2	12135.355	0.000
2	1	1	0	2	1	0	1	1	1	12650.840	0.000
2	1	1	0	3	1	0	1	1	2	12651.224	0.003
2	1	1	0	1	1	0	1	1	0	12652.001	0.000
3	0	3	1	2	2	0	2	1	2	12800.032	0.000
3	0	3	1	4	2	0	2	1	3	12800.926	0.000
3	0	3	1	3	2	0	2	1	2	12800.961	-0.002
3	0	3	1	2	2	0	2	1	1	12801.047	-0.001
3	0	3	1	3	2	0	2	1	3	12801.614	-0.002
3	0	3	0	2	2	0	2	0	2	12803.087	0.000
3	0	3	0	4	2	0	2	0	3	12803.983	0.002
3	0	3	0	3	2	0	2	0	2	12804.018	0.000
3	0	3	0	2	2	0	2	0	1	12804.104	0.001
3	0	3	0	3	2	0	2	0	3	12804.673	0.001
2	1	2	0	1	1	0	1	0	1	12931.698	0.000
2	1	2	0	2	1	0	1	0	1	12932.358	-0.001
2	1	2	0	3	1	0	1	0	2	12932.535	-0.001

2	1	2	0	2	1	0	1	0	2	12932.961	-0.001
2	1	2	1	1	1	0	1	1	1	12933.772	-0.002
2	1	2	1	2	1	0	1	1	1	12934.437	0.002
2	1	2	1	3	1	0	1	1	2	12934.611	0.000
2	1	2	1	2	1	0	1	1	2	12935.039	0.002
3	1	2	1	2	2	1	1	1	1	13756.636	-0.003
3	1	2	1	4	2	1	1	1	3	13756.657	0.001
3	1	2	1	3	2	1	1	1	2	13756.835	0.000
3	1	2	0	2	2	1	1	0	1	13763.141	-0.005
3	1	2	0	4	2	1	1	0	3	13763.164	0.001
3	1	2	0	3	2	1	1	0	2	13763.345	0.004
4	1	4	1	5	3	1	3	1	4	16131.738	0.001
4	1	4	1	3	3	1	3	1	2	16131.775	0.003
4	1	4	1	4	3	1	3	1	3	16131.824	0.000
4	1	4	0	5	3	1	3	0	4	16134.197	-0.001
4	1	4	0	3	3	1	3	0	2	16134.234	0.002
4	1	4	0	4	3	1	3	0	3	16134.282	-0.002
3	1	3	1	3	2	0	2	1	2	16461.634	-0.001
3	1	3	1	4	2	0	2	1	3	16461.677	0.000
3	1	3	1	2	2	0	2	1	1	16461.826	0.001
4	0	4	1	5	3	0	3	1	4	16879.519	0.000
4	0	4	1	4	3	0	3	1	3	16879.550	-0.001
4	0	4	1	3	3	0	3	1	2	16879.573	-0.001
4	0	4	0	5	3	0	3	0	4	16882.800	0.000
4	0	4	0	4	3	0	3	0	3	16882.831	-0.001
4	0	4	0	3	3	0	3	0	2	16882.854	-0.001
4	1	3	1	5	3	1	2	1	4	18285.813	0.002
4	1	3	1	3	3	1	2	1	2	18285.830	0.004
4	1	3	1	4	3	1	2	1	3	18285.894	0.001
4	1	3	0	5	3	1	2	0	4	18292.296	-0.002
4	1	3	0	3	3	1	2	0	2	18292.314	0.001
4	1	3	0	4	3	1	2	0	3	18292.377	-0.003

*Note that, label ‘V’ represents the tunneling state, 0 for 0^+ and 1 for 0^- state.

Table S15. Assigned transitions for the ^{13}C5 species of conf. **I**.

J”	K_a”	K_c”	V"	F”	J’	K_a’	K_c’	V'	F”	ν_{obs} /MHz	$\nu_{obs - calc}$/MHz
1	1	0	0	2	1	0	1	0	2	5497.624	0.000
1	1	0	1	2	1	0	1	1	2	5499.328	0.002
2	1	1	0	2	2	0	2	0	2	6066.915	-0.002
2	1	1	0	3	2	0	2	0	3	6067.353	0.002
2	1	1	0	1	2	0	2	0	1	6067.594	0.002

2	1	1	1	2	2	0	2	1	2	6067.987	0.000
2	1	1	1	3	2	0	2	1	3	6068.420	-0.001
2	1	1	1	1	2	0	2	1	1	6068.660	-0.002
3	1	2	1	3	3	0	3	1	3	6993.987	0.001
3	1	2	1	4	3	0	3	1	4	6994.282	0.000
3	1	2	1	2	3	0	3	1	2	6994.385	-0.001
3	1	2	0	3	3	0	3	0	3	6996.085	0.001
3	1	2	0	4	3	0	3	0	4	6996.379	-0.001
3	1	2	0	2	3	0	3	0	2	6996.481	-0.002
2	0	2	1	1	1	0	1	1	1	8586.996	0.001
2	0	2	1	3	1	0	1	1	2	8587.947	-0.001
2	0	2	1	1	1	0	1	1	0	8588.479	-0.001
2	0	2	1	2	1	0	1	1	2	8588.590	-0.002
2	0	2	0	1	1	0	1	0	1	8589.422	0.001
2	0	2	0	3	1	0	1	0	2	8590.375	0.001
2	0	2	0	1	1	0	1	0	0	8590.908	0.002
2	0	2	0	2	1	0	1	0	2	8591.020	0.001
2	1	1	1	1	1	1	0	1	0	9156.328	-0.002
2	1	1	1	3	1	1	0	1	2	9157.042	-0.001
2	1	1	1	2	1	1	0	1	1	9157.650	-0.001
2	1	1	0	1	1	1	0	0	0	9159.390	0.001
2	1	1	0	3	1	1	0	0	2	9160.103	0.002
2	1	1	0	2	1	1	0	0	1	9160.710	0.000
1	1	1	0	1	0	0	0	0	1	9282.704	0.001
1	1	1	0	2	0	0	0	0	1	9282.901	0.001
1	1	1	0	0	0	0	0	0	1	9283.196	0.001
1	1	1	1	1	0	0	0	1	1	9284.177	-0.001
1	1	1	1	2	0	0	0	1	1	9284.374	-0.001
1	1	1	1	0	0	0	0	1	1	9284.669	-0.001
1	1	0	1	2	0	0	0	0	1	11742.958	0.001
3	1	3	1	4	2	1	2	1	3	12123.813	0.002
3	1	3	1	3	2	1	2	1	2	12123.993	-0.002
3	1	3	0	4	2	1	2	0	3	12126.997	0.001
3	1	3	0	3	2	1	2	0	2	12127.180	0.001
2	1	1	0	2	1	0	1	1	1	12728.962	0.000
2	1	1	0	3	1	0	1	1	2	12729.346	0.001
2	1	1	0	1	1	0	1	1	0	12730.118	-0.001
3	0	3	1	2	2	0	2	1	2	12782.418	0.000
3	0	3	1	4	2	0	2	1	3	12783.301	0.000
3	0	3	1	3	2	0	2	1	2	12783.335	-0.002

3	0	3	1	2	2	0	2	1	1	12783.420	0.000
3	0	3	1	3	2	0	2	1	3	12783.981	-0.002
3	0	3	0	2	2	0	2	0	2	12785.566	0.000
3	0	3	0	4	2	0	2	0	3	12786.451	0.001
3	0	3	0	3	2	0	2	0	2	12786.486	-0.001
3	0	3	0	2	2	0	2	0	1	12786.570	0.001
3	0	3	0	3	2	0	2	0	3	12787.132	0.001
2	1	2	0	1	1	0	1	0	1	13067.689	0.000
2	1	2	0	2	1	0	1	0	1	13068.350	-0.001
2	1	2	0	3	1	0	1	0	2	13068.520	0.000
2	1	2	0	2	1	0	1	0	2	13068.946	0.001
2	1	2	1	1	1	0	1	1	1	13069.574	-0.001
2	1	2	1	2	1	0	1	1	1	13070.239	0.002
2	1	2	1	3	1	0	1	1	2	13070.405	-0.001
2	1	2	1	2	1	0	1	1	2	13070.833	0.002
3	1	2	1	2	2	1	1	1	1	13709.140	-0.003
3	1	2	1	4	2	1	1	1	3	13709.162	0.001
3	1	2	1	3	2	1	1	1	2	13709.337	0.000
3	1	2	0	4	2	1	1	0	3	13715.477	-0.001
3	1	2	0	3	2	1	1	0	2	13715.655	0.002
4	1	4	1	5	3	1	3	1	4	16123.850	0.000
4	1	4	1	3	3	1	3	1	2	16123.887	0.002
4	1	4	1	4	3	1	3	1	3	16123.935	0.000
4	1	4	0	5	3	1	3	0	4	16126.393	0.000
4	1	4	0	3	3	1	3	0	2	16126.430	0.002
4	1	4	0	4	3	1	3	0	3	16126.477	-0.001
3	1	3	0	3	2	0	2	0	2	16605.104	-0.002
3	1	3	0	4	2	0	2	0	3	16605.141	0.000
3	1	3	0	2	2	0	2	0	1	16605.284	-0.002
3	1	3	1	3	2	0	2	1	2	16606.232	-0.002
3	1	3	1	4	2	0	2	1	3	16606.270	0.001
3	1	3	1	2	2	0	2	1	1	16606.415	0.001
4	0	4	1	5	3	0	3	1	4	16868.551	0.000
4	0	4	1	4	3	0	3	1	3	16868.582	-0.001
4	0	4	1	3	3	0	3	1	2	16868.605	-0.001
4	0	4	0	5	3	0	3	0	4	16871.979	0.000
4	0	4	0	4	3	0	3	0	3	16872.011	-0.001
4	0	4	0	3	3	0	3	0	2	16872.034	-0.001
4	1	3	1	5	3	1	2	1	4	18226.751	0.002
4	1	3	1	3	3	1	2	1	2	18226.768	0.004

4	1	3	1	4	3	1	2	1	3	18226.8309	0.001
4	1	3	0	5	3	1	2	0	4	18233.3404	-0.002
4	1	3	0	3	3	1	2	0	2	18233.3580	0.000
4	1	3	0	4	3	1	2	0	3	18233.4196	-0.004

*Note that, label 'V' represents the tunneling state, 0 for 0^+ and 1 for 0^- state.

Table S16. Assigned transitions for the ^{15}N4 species of conf. **I**.

J''	K_a''	K_c''	V''	J'	K_a'	K_c'	V'	ν_{obs} /MHz	$\nu_{obs - calc}$/MHz
3	1	2	1	3	0	3	1	6942.328	-0.001
3	1	2	0	3	0	3	0	6944.228	0.000
2	1	2	0	1	1	1	0	8138.074	0.000
2	1	2	1	1	1	1	1	8140.076	0.000
4	1	3	1	4	0	4	1	8336.606	0.001
4	1	3	0	4	0	4	0	8341.470	0.000
2	0	2	1	1	0	1	1	8633.101	-0.001
2	0	2	0	1	0	1	0	8635.250	0.001
1	1	1	0	0	0	0	0	9209.933	0.000
1	1	1	1	0	0	0	1	9211.258	-0.001
2	1	1	0	1	1	0	0	9214.534	0.000
2	1	1	1	1	1	0	1	9214.595	-0.001
1	1	0	1	0	0	0	0	11423.931	0.001
3	1	3	1	2	1	2	1	12175.784	0.000
3	1	3	0	2	1	2	0	12181.335	0.001
3	0	3	1	2	0	2	1	12845.475	-0.001
3	0	3	0	2	0	2	0	12848.250	0.001
2	1	1	0	1	0	1	1	12952.919	0.001
2	1	2	0	1	0	1	0	13009.106	0.000
2	1	2	1	1	0	1	1	13013.606	0.001
3	1	2	1	2	1	1	1	13793.846	-0.001
3	1	2	0	2	1	1	0	13802.241	0.000
4	1	4	1	3	1	3	1	16194.282	0.001
4	1	4	0	3	1	3	0	16196.555	0.000
3	1	3	0	2	0	2	0	16555.190	-0.001
3	1	3	1	2	0	2	1	16556.288	0.000
4	0	4	1	3	0	3	1	16942.244	-0.001
4	0	4	0	3	0	3	0	16945.238	0.000
4	1	3	1	3	1	2	1	18336.522	0.002
4	1	3	0	3	1	2	0	18342.478	-0.001

*Note that, label 'V' represents the tunneling state, 0 for 0^+ and 1 for 0^- state.

Appendix IV: Kraitchman coordinates for conf. **I** and conf. **III**.

Table S17. Kraitchman coordinates of conf. **I** along with their uncertainties.

Atom	X	dX	Y	dY	Z	dZ
^{13}C1	-1.52437	0.00098	-1.31762	0.00114	0.11166	0.01345
^{13}C2	-1.82569	0.00082	-0.05017	0.00869	-0.19044	0.00789
^{13}C3	-0.87742	0.00171	1.11829	0.00134	-0.10204	0.01471
^{14}N	0.44867	0.00336	0.79297	0.00190	0.37075	0.00406
^{13}C5	1.33531	0.00112	0.07806	0.01923	0.04454	0.03371

Table S18. Kraitchman coordinates of conf. **III** along with their uncertainties.

Atom	X	dX	Y	dY	Z	dZ
^{13}C1	2.33259	0.00064	-0.88884	0.00169	0.23746	0.00633
^{13}C2	1.47343	0.00102	-0.15885	0.00945	-0.45761	0.00328
^{13}C3	0.75070	0.00200	1.04276	0.00144	0.10570	0.01420
^{14}N	-0.63952	0.00236	0.93425	0.00162	-0.15810	0.00957
^{13}C5	-1.44586	0.00104	0.03717	0.04039	-0.03287	0.04567