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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. Ia | | | |
|---|-----------|-----------|-----------|
| 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. Ib | | | |
| 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.

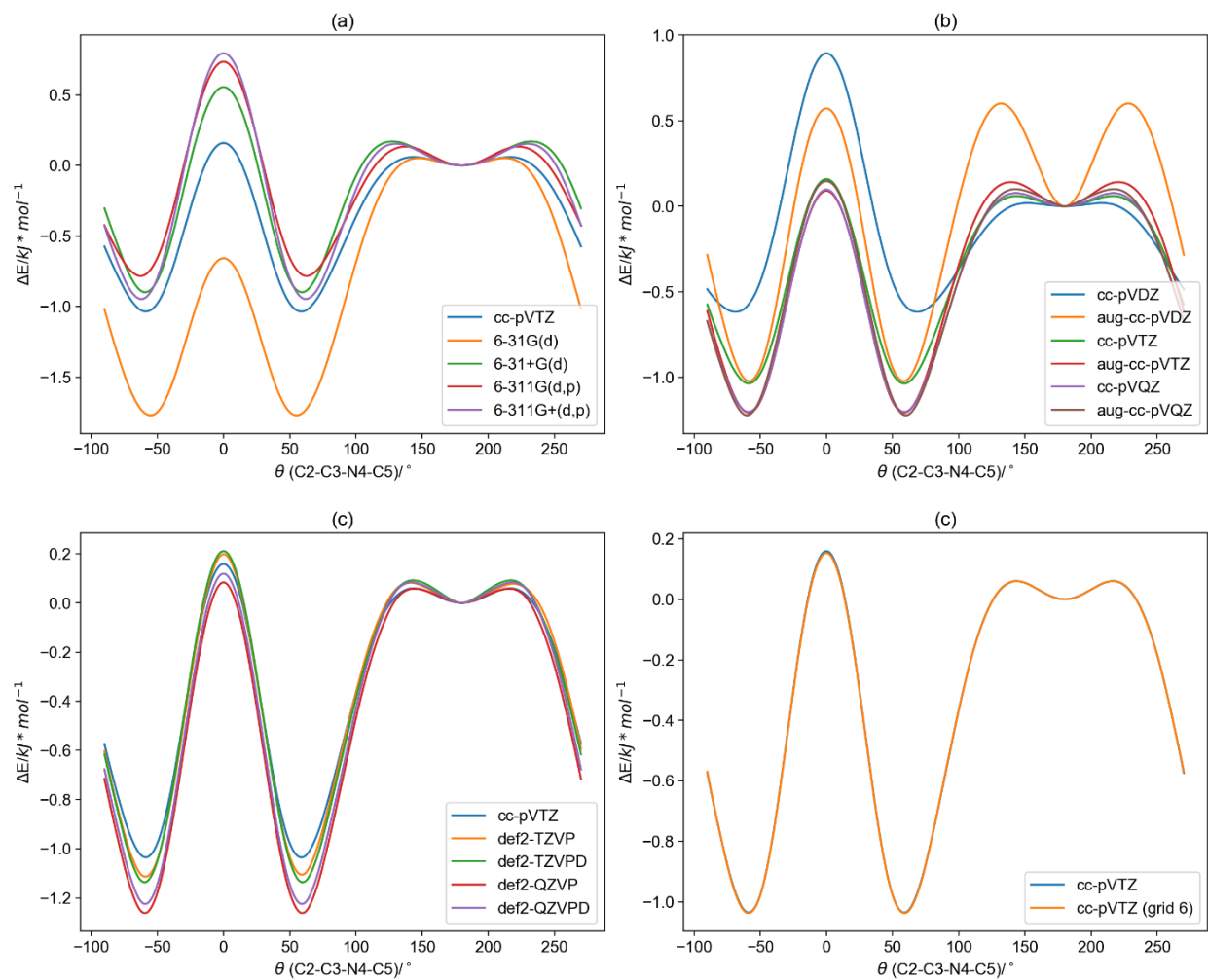


FIG. S1. Potential energy profiles of Route 1 calculated using the B3LYP-D3(BJ) method and different types of basis set: (a). Pople's basis sets, (b). Dunning's basis sets, (c). Karlsruhe's basis sets, (d) integration grid. The default grid 4 was used if not mentioned otherwise.

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' | $\nu_{\text{obs}}/\text{MHz}$ | $\nu_{\text{obs}} - \nu_{\text{calc}}/\text{MHz}$ |
|-------|---------|---------|-------|------|--------|--------|------|-------------------------------|---|
| 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 $^{13}\text{C1}$ species of conf. **III**.

| J'' | K_a'' | K_c'' | F'' | J' | K_a' | K_c' | F' | $\nu_{\text{obs}}/\text{MHz}$ | $\nu_{\text{obs}} - \nu_{\text{calc}}/\text{MHz}$ |
|-------|---------|---------|-------|------|--------|--------|------|-------------------------------|---|
| 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 $^{13}\text{C}_2$ species of conf. **III**.

| J'' | K_a'' | K_c'' | F'' | J' | K_a' | K_c' | F' | $\nu_{\text{obs}}/\text{MHz}$ | $\nu_{\text{obs}} - \nu_{\text{calc}}/\text{MHz}$ |
|-------|---------|---------|-------|------|--------|--------|------|-------------------------------|---|
| 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 $^{13}\text{C3}$ species of conf. **III**.

| J'' | K_a'' | K_c'' | F'' | J' | K_a' | K_c' | F' | $\nu_{\text{obs}}/\text{MHz}$ | $\nu_{\text{obs}} - \nu_{\text{calc}}/\text{MHz}$ |
|-------|---------|---------|-------|------|--------|--------|------|-------------------------------|---|
| 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 $^{15}\text{N}_4$ species of conf. **III**.

| J'' | K_a'' | K_c'' | J' | K_a' | K_c' | $\nu_{\text{obs}}/\text{MHz}$ | $\nu_{\text{obs}} - \nu_{\text{calc}}/\text{MHz}$ |
|-------|---------|---------|------|--------|--------|-------------------------------|---|
| 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 $^{13}\text{C}_5$ species of conf. **III**.

| J'' | K_a'' | K_c'' | F'' | J' | K_a' | K_c' | F' | $\nu_{\text{obs}}/\text{MHz}$ | $\nu_{\text{obs}} - \nu_{\text{calc}}/\text{MHz}$ |
|-------|---------|---------|-------|------|--------|--------|------|-------------------------------|---|
| 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 $^{18}\text{O}_6$ species of conf. **III**.

| J'' | K_a'' | K_c'' | F'' | J' | K_a' | K_c' | F' | $\nu_{\text{obs}}/\text{MHz}$ | $\nu_{\text{obs}} - \nu_{\text{calc}}/\text{MHz}$ |
|-------|---------|---------|-------|------|--------|--------|------|-------------------------------|---|
| 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'' | $\nu_{\text{obs}}/\text{MHz}$ | $\nu_{\text{obs}} - \nu_{\text{calc}}/\text{MHz}$ |
|-------|---------|---------|-------|-------|------|--------|--------|------|-------|-------------------------------|---|
| 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 ¹³C1 species of conf. I.

| J'' | K _a '' | K _c '' | V'' | F'' | J' | K _a ' | K _c ' | V' | F' | V _{obs} /MHz | V _{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 ¹³C2 species of conf. I.

| J'' | K _a '' | K _c '' | V'' | F'' | J' | K _a ' | K _c ' | V' | F' | V _{obs} /MHz | V _{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 ¹³C₃ species of conf. I.

| J'' | K _a '' | K _c '' | V'' | F'' | J' | K _a ' | K _c ' | V' | F' | V _{obs} /MHz | V _{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 ¹³C5 species of conf. I.

| J'' | K _a '' | K _c '' | V'' | F'' | J' | K _a ' | K _c ' | V' | F' | V _{obs} /MHz | V _{obs} - cal/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 ¹⁵N₄ species of conf. I.

| J'' | K _a '' | K _c '' | V'' | J' | K _a ' | K _c ' | V' | V _{obs} /MHz | V _{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 |