



## Supporting Information

for

### **Conformational signature of Ishikawa's reagent using NMR information from diastereotopic fluorines**

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### **Standard coordinates for the geometries of conformers of 1, NMR spectra and tables containing calculated spectroscopic data**

## Contents

Pages S2–S15. Standard coordinates for the conformers of **1**, optimized in implicit cyclohexane, chloroform and pyridine solvents at the  $\omega$ B97X-D/6-311++g(d,p) level.

Page S16. Table S1. Calculated [ $\omega$ B97X-D/6-311++g(d,p)] spin–spin coupling constants and F–C–C–F dihedral angles, in implicit cyclohexane solvent.

Page S17. Table S2. Calculated [ $\omega$ B97X-D/6-311++g(d,p)] spin–spin coupling constants and F–C–C–F dihedral angles, in implicit pyridine solvent.

Page S18. Table S3. Calculated  $^3J_{\text{H2,F1}}$  coupling constants (in Hz) and H–C–C–F(1) dihedral angles (in degrees) for the optimized geometries of **1**.

Page S19. Table S4. Relative nuclear-electronic energies (in kcal mol<sup>−1</sup> and population % in parenthesis) and molecular dipole moments (in D) for the conformers of **1**, calculated at the MP2/6-311++g(d,p) level.

Page S20–S31. Figures S1 to S12. <sup>1</sup>H, <sup>19</sup>F and <sup>13</sup>C NMR spectra for **1**, in C<sub>6</sub>D<sub>12</sub>, CDCl<sub>3</sub> and C<sub>5</sub>D<sub>5</sub>N solutions.

**1Aa\_C<sub>6</sub>H<sub>12</sub>\_ωB97X-D/6-311++G(d,p) E= -927.1983983**

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -2.678614               | 0.940613  | 0.000000  |
| 2                | 1                | 0              | -3.035286               | 0.437909  | -0.874628 |
| 3                | 1                | 0              | -3.035287               | 0.434522  | 0.872672  |
| 4                | 6                | 0              | -0.625272               | 1.666550  | 1.257405  |
| 5                | 1                | 0              | -0.982252               | 1.162369  | 2.131056  |
| 6                | 1                | 0              | 0.444728                | 1.666211  | 1.257593  |
| 7                | 6                | 0              | -0.625298               | -0.511338 | 0.000000  |
| 8                | 9                | 0              | 0.724702                | -0.511354 | -0.000321 |
| 9                | 9                | 0              | -1.075568               | -1.147821 | -1.102110 |
| 10               | 7                | 0              | -1.138614               | 0.940594  | 0.000000  |
| 11               | 6                | 0              | -1.138341               | -1.237189 | 1.257588  |
| 12               | 1                | 0              | -0.800791               | -2.252486 | 1.246050  |
| 13               | 6                | 0              | -2.677974               | -1.208267 | 1.274786  |
| 14               | 9                | 0              | -3.155545               | -2.351529 | 0.738709  |
| 15               | 9                | 0              | -3.116365               | -0.155196 | 0.552737  |
| 16               | 9                | 0              | -3.111688               | -1.092723 | 2.547987  |
| 17               | 9                | 0              | -0.664291               | -0.617860 | 2.359498  |
| 18               | 6                | 0              | -1.138144               | 3.118639  | 1.257135  |
| 19               | 1                | 0              | -0.526904               | 3.712907  | 1.903765  |
| 20               | 1                | 0              | -1.093817               | 3.512370  | 0.263197  |
| 21               | 1                | 0              | -2.150059               | 3.139559  | 1.604254  |
| 22               | 6                | 0              | -3.191929               | 2.392543  | 0.002816  |
| 23               | 1                | 0              | -3.345348               | 2.714647  | 1.011583  |
| 24               | 1                | 0              | -2.470399               | 3.026847  | -0.468303 |
| 25               | 1                | 0              | -4.116693               | 2.444942  | -0.532876 |

**1Ab\_C<sub>6</sub>H<sub>12</sub>\_ωB97X-D/6-311++G(d,p) E = -927.2009632**

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -3.479231               | 0.094755  | 1.224585  |
| 2                | 1                | 0              | -3.685767               | -0.666872 | 0.475765  |
| 3                | 1                | 0              | -4.161005               | -0.095768 | 2.064559  |
| 4                | 6                | 0              | -1.731559               | 0.814619  | 2.826838  |
| 5                | 1                | 0              | -2.653831               | 1.264804  | 3.203321  |
| 6                | 1                | 0              | -1.341882               | 0.201117  | 3.641905  |
| 7                | 6                | 0              | -1.551998               | -1.319250 | 1.702217  |
| 8                | 9                | 0              | -2.171328               | -2.166364 | 2.625095  |
| 9                | 9                | 0              | -0.254985               | -1.260706 | 2.124186  |
| 10               | 7                | 0              | -2.087412               | -0.038359 | 1.675851  |
| 11               | 6                | 0              | -1.512034               | -2.135172 | 0.388218  |
| 12               | 1                | 0              | -0.823070               | -2.963043 | 0.569033  |
| 13               | 6                | 0              | -1.001501               | -1.373366 | -0.841916 |
| 14               | 9                | 0              | 0.145841                | -0.746374 | -0.580681 |
| 15               | 9                | 0              | -1.879071               | -0.475915 | -1.293900 |
| 16               | 9                | 0              | -0.775954               | -2.243769 | -1.836652 |
| 17               | 9                | 0              | -2.739654               | -2.658827 | 0.071526  |
| 18               | 6                | 0              | -0.727793               | 1.894810  | 2.451302  |
| 19               | 1                | 0              | -0.514930               | 2.532609  | 3.313744  |
| 20               | 1                | 0              | 0.208175                | 1.446750  | 2.112669  |
| 21               | 1                | 0              | -1.116452               | 2.520122  | 1.644373  |
| 22               | 6                | 0              | -3.746878               | 1.467877  | 0.626207  |
| 23               | 1                | 0              | -3.601070               | 2.266201  | 1.357978  |
| 24               | 1                | 0              | -3.083505               | 1.651443  | -0.220769 |
| 25               | 1                | 0              | -4.781008               | 1.522310  | 0.278336  |

**1Ac\_C<sub>6</sub>H<sub>12</sub>\_ωB97X-D/6-311++G(d,p) E = -927.1943787**

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -2.606598               | -0.470148 | -0.032288 |
| 2                | 1                | 0              | -3.324306               | 0.085095  | -0.641089 |
| 3                | 1                | 0              | -2.655082               | -1.504220 | -0.372813 |
| 4                | 6                | 0              | -0.974729               | 1.424767  | 0.008464  |
| 5                | 1                | 0              | -0.893767               | 1.555692  | 1.094697  |
| 6                | 1                | 0              | -0.015208               | 1.694459  | -0.426138 |
| 7                | 6                | 0              | -0.276469               | -0.920194 | -0.418651 |
| 8                | 9                | 0              | -0.573945               | -1.820960 | -1.422474 |
| 9                | 9                | 0              | -0.193964               | -1.751554 | 0.704057  |
| 10               | 7                | 0              | -1.264907               | 0.035757  | -0.342199 |
| 11               | 6                | 0              | 1.180860                | -0.495927 | -0.686365 |
| 12               | 1                | 0              | 1.706904                | -1.434482 | -0.867625 |
| 13               | 6                | 0              | 1.957506                | 0.221358  | 0.458263  |
| 14               | 9                | 0              | 3.123830                | -0.408251 | 0.658735  |
| 15               | 9                | 0              | 1.305174                | 0.230373  | 1.621464  |
| 16               | 9                | 0              | 2.238807                | 1.486030  | 0.139419  |
| 17               | 9                | 0              | 1.257107                | 0.263645  | -1.820959 |
| 18               | 6                | 0              | -2.014405               | 2.385469  | -0.553928 |
| 19               | 1                | 0              | -1.686728               | 3.412076  | -0.376686 |
| 20               | 1                | 0              | -2.131275               | 2.240053  | -1.630281 |
| 21               | 1                | 0              | -2.990519               | 2.266727  | -0.078475 |
| 22               | 6                | 0              | -2.983706               | -0.386857 | 1.444469  |
| 23               | 1                | 0              | -2.276918               | -0.947939 | 2.058102  |
| 24               | 1                | 0              | -3.005602               | 0.646493  | 1.800806  |
| 25               | 1                | 0              | -3.980992               | -0.808614 | 1.592929  |

**1Ba\_C<sub>6</sub>H<sub>12</sub>\_ωB97X-D/6-311++G(d,p) E = -927.1975755**

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -2.289275               | 1.102516  | 0.808931  |
| 2                | 1                | 0              | -2.080364               | 0.611894  | -0.139235 |
| 3                | 1                | 0              | -3.247826               | 0.709787  | 1.168647  |
| 4                | 6                | 0              | -1.326892               | 1.290554  | 3.103948  |
| 5                | 1                | 0              | -0.500473               | 0.885183  | 3.689225  |
| 6                | 1                | 0              | -1.156100               | 2.369708  | 3.066330  |
| 7                | 6                | 0              | -0.534332               | -0.450748 | 1.589693  |
| 8                | 9                | 0              | 0.712898                | -0.357321 | 2.154214  |
| 9                | 9                | 0              | -0.347913               | -0.714904 | 0.272202  |
| 10               | 7                | 0              | -1.203797               | 0.772819  | 1.737689  |
| 11               | 6                | 0              | -1.194128               | -1.684802 | 2.257290  |
| 12               | 1                | 0              | -1.167098               | -1.540410 | 3.340300  |
| 13               | 6                | 0              | -0.573707               | -3.057089 | 1.965390  |
| 14               | 9                | 0              | 0.713348                | -3.089094 | 2.317218  |
| 15               | 9                | 0              | -0.670239               | -3.405471 | 0.684146  |
| 16               | 9                | 0              | -1.214696               | -3.991494 | 2.686005  |
| 17               | 9                | 0              | -2.506710               | -1.744947 | 1.850215  |
| 18               | 6                | 0              | -2.656905               | 1.013227  | 3.805369  |
| 19               | 1                | 0              | -2.608956               | 1.390026  | 4.829759  |
| 20               | 1                | 0              | -3.488866               | 1.516434  | 3.307500  |
| 21               | 1                | 0              | -2.891395               | -0.053058 | 3.846112  |
| 22               | 6                | 0              | -2.390431               | 2.605025  | 0.583661  |
| 23               | 1                | 0              | -2.679154               | 3.138330  | 1.493143  |
| 24               | 1                | 0              | -1.435800               | 3.006430  | 0.236286  |
| 25               | 1                | 0              | -3.150998               | 2.810819  | -0.172995 |

**1Bb\_C<sub>6</sub>H<sub>12</sub>\_ωB97X-D/6-311++G(d,p) E = -927.1988454**

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -3.435396               | 0.653620  | 1.502306  |
| 2                | 1                | 0              | -3.735065               | 0.088614  | 0.620127  |
| 3                | 1                | 0              | -4.183702               | 0.451103  | 2.281252  |
| 4                | 6                | 0              | -1.642429               | 0.775815  | 3.213283  |
| 5                | 1                | 0              | -2.491993               | 1.277385  | 3.685535  |
| 6                | 1                | 0              | -1.348179               | -0.024632 | 3.895247  |
| 7                | 6                | 0              | -1.789423               | -1.135074 | 1.745163  |
| 8                | 9                | 0              | -2.498388               | -2.014651 | 2.579892  |
| 9                | 9                | 0              | -0.487966               | -1.338456 | 2.087180  |
| 10               | 7                | 0              | -2.114692               | 0.196779  | 1.941806  |
| 11               | 6                | 0              | -2.049965               | -1.664721 | 0.316554  |
| 12               | 1                | 0              | -3.112312               | -1.891258 | 0.209934  |
| 13               | 6                | 0              | -1.283702               | -2.948656 | -0.042667 |
| 14               | 9                | 0              | -1.473629               | -3.906686 | 0.864557  |
| 15               | 9                | 0              | 0.023835                | -2.742556 | -0.177228 |
| 16               | 9                | 0              | -1.740834               | -3.405844 | -1.219720 |
| 17               | 9                | 0              | -1.697676               | -0.721680 | -0.613185 |
| 18               | 6                | 0              | -0.488045               | 1.748495  | 3.018521  |
| 19               | 1                | 0              | -0.183058               | 2.170050  | 3.980321  |
| 20               | 1                | 0              | 0.369814                | 1.238399  | 2.576902  |
| 21               | 1                | 0              | -0.774643               | 2.568494  | 2.356660  |
| 22               | 6                | 0              | -3.435866               | 2.131843  | 1.140634  |
| 23               | 1                | 0              | -3.203849               | 2.761129  | 2.002938  |
| 24               | 1                | 0              | -2.701269               | 2.332355  | 0.358009  |
| 25               | 1                | 0              | -4.424748               | 2.420419  | 0.777077  |

**1Bc\_C<sub>6</sub>H<sub>12</sub>\_ωB97X-D/6-311++G(d,p) E = -927.198922**

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -3.666243               | -0.190422 | 1.421050  |
| 2                | 1                | 0              | -3.940250               | -1.238865 | 1.306997  |
| 3                | 1                | 0              | -4.250499               | 0.191301  | 2.264692  |
| 4                | 6                | 0              | -1.843276               | 1.071731  | 2.522350  |
| 5                | 1                | 0              | -0.769318               | 1.239451  | 2.415423  |
| 6                | 1                | 0              | -2.324447               | 1.925861  | 2.040264  |
| 7                | 6                | 0              | -1.582799               | -1.312833 | 1.938149  |
| 8                | 9                | 0              | -1.834764               | -2.142178 | 0.878309  |
| 9                | 9                | 0              | -2.054646               | -2.026145 | 3.034579  |
| 10               | 7                | 0              | -2.231348               | -0.101598 | 1.734647  |
| 11               | 6                | 0              | -0.048577               | -1.194647 | 2.088681  |
| 12               | 1                | 0              | 0.319391                | -0.431629 | 1.399480  |
| 13               | 6                | 0              | 0.729492                | -2.484487 | 1.774737  |
| 14               | 9                | 0              | 0.734229                | -2.724191 | 0.460190  |
| 15               | 9                | 0              | 0.251450                | -3.558505 | 2.398479  |
| 16               | 9                | 0              | 2.002565                | -2.323069 | 2.158393  |
| 17               | 9                | 0              | 0.266423                | -0.828422 | 3.372423  |
| 18               | 6                | 0              | -2.219265               | 1.031841  | 4.002955  |
| 19               | 1                | 0              | -1.950604               | 1.981396  | 4.472619  |
| 20               | 1                | 0              | -3.292890               | 0.883570  | 4.139258  |
| 21               | 1                | 0              | -1.693950               | 0.231053  | 4.523650  |
| 22               | 6                | 0              | -4.006681               | 0.570220  | 0.146925  |
| 23               | 1                | 0              | -3.729403               | 1.624776  | 0.224695  |
| 24               | 1                | 0              | -3.478012               | 0.138874  | -0.705491 |
| 25               | 1                | 0              | -5.081382               | 0.520679  | -0.046338 |

**1Ca\_C<sub>6</sub>H<sub>12</sub>\_ωB97X-D/6-311++G(d,p) E = -927.1949454**

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -1.665312               | -1.372149 | -0.844694 |
| 2                | 1                | 0              | -2.704198               | -1.244634 | -1.167493 |
| 3                | 1                | 0              | -1.056658               | -1.349149 | -1.747381 |
| 4                | 6                | 0              | -2.424695               | 0.286849  | 0.809223  |
| 5                | 1                | 0              | -3.075880               | 0.914894  | 0.183562  |
| 6                | 1                | 0              | -3.020594               | -0.586483 | 1.081546  |
| 7                | 6                | 0              | -0.278112               | 0.623045  | -0.378183 |
| 8                | 9                | 0              | 0.633689                | -0.053882 | -1.118184 |
| 9                | 9                | 0              | 0.406738                | 1.088317  | 0.720132  |
| 10               | 7                | 0              | -1.302057               | -0.245921 | 0.028156  |
| 11               | 6                | 0              | -0.671428               | 1.911788  | -1.144667 |
| 12               | 1                | 0              | -1.331151               | 2.506040  | -0.507097 |
| 13               | 6                | 0              | -1.399857               | 1.699992  | -2.476780 |
| 14               | 9                | 0              | -2.607256               | 1.150844  | -2.272302 |
| 15               | 9                | 0              | -0.731648               | 0.917394  | -3.323195 |
| 16               | 9                | 0              | -1.592123               | 2.879246  | -3.075271 |
| 17               | 9                | 0              | 0.454895                | 2.646880  | -1.411654 |
| 18               | 6                | 0              | -2.056677               | 1.024050  | 2.090156  |
| 19               | 1                | 0              | -2.974211               | 1.233985  | 2.645158  |
| 20               | 1                | 0              | -1.400970               | 0.414419  | 2.713888  |
| 21               | 1                | 0              | -1.556492               | 1.975483  | 1.903948  |
| 22               | 6                | 0              | -1.485482               | -2.709993 | -0.140631 |
| 23               | 1                | 0              | -0.434705               | -2.870030 | 0.108858  |
| 24               | 1                | 0              | -2.066116               | -2.750767 | 0.784968  |
| 25               | 1                | 0              | -1.820260               | -3.525777 | -0.787058 |

**1Cb\_C<sub>6</sub>H<sub>12</sub>\_ωB97X-D/6-311++G(d,p) E = -927.1947101**

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 7                | 0              | -1.796216               | 2.212106  | 1.733944  |
| 2                | 6                | 0              | -1.203616               | 3.190292  | 2.664365  |
| 3                | 1                | 0              | -0.684881               | 2.689038  | 3.485550  |
| 4                | 1                | 0              | -2.035331               | 3.731822  | 3.116805  |
| 5                | 6                | 0              | -0.280374               | 4.175768  | 1.962729  |
| 6                | 1                | 0              | 0.101055                | 4.912991  | 2.674375  |
| 7                | 1                | 0              | -0.820634               | 4.702493  | 1.172197  |
| 8                | 1                | 0              | 0.574545                | 3.664561  | 1.515246  |
| 9                | 6                | 0              | -3.963644               | 3.326821  | 1.263202  |
| 10               | 1                | 0              | -3.690506               | 3.487423  | 0.219609  |
| 11               | 1                | 0              | -3.713889               | 4.230046  | 1.825312  |
| 12               | 1                | 0              | -5.046024               | 3.189877  | 1.324018  |
| 13               | 6                | 0              | -3.259678               | 2.098722  | 1.821575  |
| 14               | 1                | 0              | -3.582851               | 1.217081  | 1.271048  |
| 15               | 1                | 0              | -3.556402               | 1.928694  | 2.864998  |
| 16               | 6                | 0              | -1.093361               | 1.008633  | 1.537353  |
| 17               | 9                | 0              | 0.173294                | 1.124631  | 2.024523  |
| 18               | 9                | 0              | -1.647934               | -0.056045 | 2.212539  |
| 19               | 6                | 0              | -0.875753               | 0.586719  | 0.062632  |
| 20               | 1                | 0              | -0.250901               | 1.357755  | -0.394826 |
| 21               | 6                | 0              | -2.096951               | 0.400008  | -0.844532 |
| 22               | 9                | 0              | -1.699259               | -0.100761 | -2.018166 |
| 23               | 9                | 0              | -3.004684               | -0.437622 | -0.335726 |
| 24               | 9                | 0              | -2.700125               | 1.568639  | -1.091502 |
| 25               | 9                | 0              | -0.193860               | -0.604297 | 0.050182  |

**1Cc\_C<sub>6</sub>H<sub>12</sub>\_ωB97X-D/6-311++G(d,p)  $E = -927.2000985$** 

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -3.639171               | 0.660171  | 1.758059  |
| 2                | 1                | 0              | -4.097733               | -0.311354 | 1.564266  |
| 3                | 1                | 0              | -4.113833               | 1.043903  | 2.665086  |
| 4                | 6                | 0              | -1.766272               | 1.045333  | 3.329580  |
| 5                | 1                | 0              | -2.361314               | 0.608673  | 4.143073  |
| 6                | 1                | 0              | -0.730229               | 0.759976  | 3.512839  |
| 7                | 6                | 0              | -1.661614               | -0.738473 | 1.673281  |
| 8                | 9                | 0              | -2.193857               | -1.139003 | 0.492779  |
| 9                | 9                | 0              | -1.980199               | -1.769605 | 2.564241  |
| 10               | 7                | 0              | -2.199669               | 0.492294  | 2.040848  |
| 11               | 6                | 0              | -0.123039               | -0.792371 | 1.540687  |
| 12               | 1                | 0              | 0.347116                | -0.711566 | 2.521762  |
| 13               | 6                | 0              | 0.486835                | 0.297651  | 0.645503  |
| 14               | 9                | 0              | 0.486178                | 1.479298  | 1.277433  |
| 15               | 9                | 0              | -0.146010               | 0.446811  | -0.515754 |
| 16               | 9                | 0              | 1.761394                | -0.011070 | 0.379634  |
| 17               | 9                | 0              | 0.210112                | -2.008472 | 1.007275  |
| 18               | 6                | 0              | -1.863632               | 2.563456  | 3.357237  |
| 19               | 1                | 0              | -1.512720               | 2.936597  | 4.322122  |
| 20               | 1                | 0              | -1.251693               | 3.001513  | 2.567087  |
| 21               | 1                | 0              | -2.893118               | 2.904115  | 3.225511  |
| 22               | 6                | 0              | -3.886595               | 1.603016  | 0.589623  |
| 23               | 1                | 0              | -3.453584               | 2.586219  | 0.787442  |
| 24               | 1                | 0              | -3.434735               | 1.207792  | -0.322001 |
| 25               | 1                | 0              | -4.960156               | 1.723118  | 0.420420  |

**1Aa\_CHCl<sub>3</sub>\_ωB97X-D/6-311++G(d,p)  $E = -927.1998691$** 

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -1.389626               | -1.291010 | 0.522379  |
| 2                | 1                | 0              | -0.496899               | -1.900119 | 0.371620  |
| 3                | 1                | 0              | -1.503975               | -1.182486 | 1.604574  |
| 4                | 6                | 0              | -1.528216               | 1.187057  | 0.829390  |
| 5                | 1                | 0              | -0.952883               | 1.135096  | 1.763576  |
| 6                | 1                | 0              | -1.230691               | 2.102389  | 0.318822  |
| 7                | 6                | 0              | -0.197062               | 0.243027  | -0.993480 |
| 8                | 9                | 0              | -0.558713               | 1.270934  | -1.833455 |
| 9                | 9                | 0              | -0.092148               | -0.873523 | -1.767513 |
| 10               | 7                | 0              | -1.192363               | 0.052933  | -0.034890 |
| 11               | 6                | 0              | 1.263075                | 0.610322  | -0.587230 |
| 12               | 1                | 0              | 1.877689                | 0.631987  | -1.489656 |
| 13               | 6                | 0              | 1.934759                | -0.328980 | 0.417150  |
| 14               | 9                | 0              | 1.977285                | -1.583427 | -0.043499 |
| 15               | 9                | 0              | 1.308922                | -0.340692 | 1.598877  |
| 16               | 9                | 0              | 3.193544                | 0.068136  | 0.635198  |
| 17               | 9                | 0              | 1.266022                | 1.861186  | -0.016913 |
| 18               | 6                | 0              | -3.017743               | 1.248078  | 1.137801  |
| 19               | 1                | 0              | -3.230371               | 2.126980  | 1.751166  |
| 20               | 1                | 0              | -3.597875               | 1.316084  | 0.214753  |
| 21               | 1                | 0              | -3.352325               | 0.367755  | 1.692130  |
| 22               | 6                | 0              | -2.595608               | -2.007679 | -0.072500 |
| 23               | 1                | 0              | -3.510648               | -1.432612 | 0.083384  |
| 24               | 1                | 0              | -2.461210               | -2.153131 | -1.146091 |
| 25               | 1                | 0              | -2.719455               | -2.988133 | 0.396221  |

**1Ab\_CHCl<sub>3</sub>\_ωB97X-D/6-311++G(d,p)  $E = -927.2024633$** 

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 1.194346                | 1.169730  | 1.120673  |
| 2                | 1                | 0              | 0.196022                | 1.346204  | 1.515064  |
| 3                | 1                | 0              | 1.834770                | 0.930827  | 1.980305  |
| 4                | 6                | 0              | 2.477797                | -0.446463 | -0.252863 |
| 5                | 1                | 0              | 3.235280                | 0.089179  | 0.324646  |
| 6                | 1                | 0              | 2.605275                | -1.503795 | -0.011472 |
| 7                | 6                | 0              | 0.234360                | -0.977331 | 0.483756  |
| 8                | 9                | 0              | 0.484065                | -1.647382 | 1.688184  |
| 9                | 9                | 0              | 0.322294                | -1.957646 | -0.462485 |
| 10               | 7                | 0              | 1.153666                | 0.022777  | 0.202214  |
| 11               | 6                | 0              | -1.267926               | -0.610279 | 0.546899  |
| 12               | 1                | 0              | -1.814237               | -1.554332 | 0.498187  |
| 13               | 6                | 0              | -1.771827               | 0.271880  | -0.602780 |
| 14               | 9                | 0              | -1.406398               | -0.222841 | -1.786358 |
| 15               | 9                | 0              | -1.336269               | 1.530106  | -0.519901 |
| 16               | 9                | 0              | -3.111886               | 0.314404  | -0.572139 |
| 17               | 9                | 0              | -1.594598               | 0.015721  | 1.723846  |
| 18               | 6                | 0              | 2.686194                | -0.216047 | -1.742564 |
| 19               | 1                | 0              | 3.686990                | -0.540913 | -2.040033 |
| 20               | 1                | 0              | 1.953036                | -0.778417 | -2.323993 |
| 21               | 1                | 0              | 2.577438                | 0.842903  | -1.987963 |
| 22               | 6                | 0              | 1.689213                | 2.430493  | 0.427958  |
| 23               | 1                | 0              | 2.707926                | 2.313595  | 0.050716  |
| 24               | 1                | 0              | 1.038993                | 2.689451  | -0.409613 |
| 25               | 1                | 0              | 1.691779                | 3.260157  | 1.138563  |

**1Ac\_CHCl<sub>3</sub>\_ωB97X-D/6-311++G(d,p)  $E = -927.1960818$** 

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 2.595521                | -0.494662 | -0.089377 |
| 2                | 1                | 0              | 3.405257                | -0.004416 | 0.456046  |
| 3                | 1                | 0              | 2.663644                | -1.554790 | 0.152078  |
| 4                | 6                | 0              | 1.009969                | 1.415383  | 0.204913  |
| 5                | 1                | 0              | 0.824757                | 1.603143  | -0.858804 |
| 6                | 1                | 0              | 0.100195                | 1.667287  | 0.744411  |
| 7                | 6                | 0              | 0.338453                | -0.940785 | 0.616777  |
| 8                | 9                | 0              | 0.782736                | -1.921904 | 1.487792  |
| 9                | 9                | 0              | 0.041068                | -1.692396 | -0.531630 |
| 10               | 7                | 0              | 1.320027                | 0.004603  | 0.444064  |
| 11               | 6                | 0              | -1.038403               | -0.518705 | 1.164325  |
| 12               | 1                | 0              | -1.542711               | -1.454141 | 1.409325  |
| 13               | 6                | 0              | -1.995193               | 0.251277  | 0.204664  |
| 14               | 9                | 0              | -3.152464               | -0.416987 | 0.103026  |
| 15               | 9                | 0              | -1.515177               | 0.397489  | -1.031959 |
| 16               | 9                | 0              | -2.276393               | 1.467204  | 0.677217  |
| 17               | 9                | 0              | -0.885384               | 0.198547  | 2.320805  |
| 18               | 6                | 0              | 2.111760                | 2.335697  | 0.712226  |
| 19               | 1                | 0              | 1.787787                | 3.372825  | 0.602801  |
| 20               | 1                | 0              | 2.317858                | 2.145608  | 1.768011  |
| 21               | 1                | 0              | 3.040596                | 2.221006  | 0.149569  |
| 22               | 6                | 0              | 2.768524                | -0.289960 | -1.591616 |
| 23               | 1                | 0              | 1.955822                | -0.763354 | -2.145829 |
| 24               | 1                | 0              | 2.796904                | 0.770002  | -1.856530 |
| 25               | 1                | 0              | 3.712394                | -0.736427 | -1.913153 |



**1Ba\_CHCl<sub>3</sub>\_ωB97X-D/6-311++G(d,p)  $E = -927.1996028$** 

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 2.225895                | -0.654591 | -0.890175 |
| 2                | 1                | 0              | 1.730604                | -1.543547 | -1.274633 |
| 3                | 1                | 0              | 2.134059                | 0.122022  | -1.658573 |
| 4                | 6                | 0              | 2.029170                | 0.968758  | 0.996996  |
| 5                | 1                | 0              | 1.364777                | 1.186859  | 1.834085  |
| 6                | 1                | 0              | 3.000280                | 0.742403  | 1.444513  |
| 7                | 6                | 0              | 0.178776                | -0.535922 | 0.486277  |
| 8                | 9                | 0              | -0.141233               | -0.584841 | 1.821369  |
| 9                | 9                | 0              | -0.091141               | -1.766700 | -0.021055 |
| 10               | 7                | 0              | 1.544405                | -0.254596 | 0.346065  |
| 11               | 6                | 0              | -0.808587               | 0.484561  | -0.135570 |
| 12               | 1                | 0              | -0.698544               | 1.434082  | 0.393547  |
| 13               | 6                | 0              | -2.298725               | 0.121501  | -0.116749 |
| 14               | 9                | 0              | -2.732867               | -0.078595 | 1.129553  |
| 15               | 9                | 0              | -2.575609               | -0.964976 | -0.837541 |
| 16               | 9                | 0              | -3.007488               | 1.136877  | -0.635244 |
| 17               | 9                | 0              | -0.460390               | 0.666867  | -1.454605 |
| 18               | 6                | 0              | 2.161655                | 2.196274  | 0.095829  |
| 19               | 1                | 0              | 2.471448                | 3.051659  | 0.700537  |
| 20               | 1                | 0              | 2.916783                | 2.049411  | -0.679586 |
| 21               | 1                | 0              | 1.222119                | 2.453896  | -0.398657 |
| 22               | 6                | 0              | 3.693984                | -0.969470 | -0.638205 |
| 23               | 1                | 0              | 4.256903                | -0.084831 | -0.329886 |
| 24               | 1                | 0              | 3.796327                | -1.731996 | 0.137317  |
| 25               | 1                | 0              | 4.148734                | -1.344808 | -1.557703 |

**1Bb\_CHCl<sub>3</sub>\_ωB97X-D/6-311++G(d,p)  $E = -927.2010029$** 

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -3.440527               | 0.652718  | 1.507899  |
| 2                | 1                | 0              | -3.745712               | 0.081941  | 0.631627  |
| 3                | 1                | 0              | -4.189464               | 0.463411  | 2.288772  |
| 4                | 6                | 0              | -1.644576               | 0.772970  | 3.219668  |
| 5                | 1                | 0              | -2.492822               | 1.274763  | 3.693577  |
| 6                | 1                | 0              | -1.344550               | -0.023394 | 3.903769  |
| 7                | 6                | 0              | -1.792695               | -1.138037 | 1.748779  |
| 8                | 9                | 0              | -2.491708               | -2.031263 | 2.581832  |
| 9                | 9                | 0              | -0.487425               | -1.338696 | 2.087268  |
| 10               | 7                | 0              | -2.122929               | 0.188545  | 1.952891  |
| 11               | 6                | 0              | -2.051461               | -1.661508 | 0.317944  |
| 12               | 1                | 0              | -3.113718               | -1.882800 | 0.204402  |
| 13               | 6                | 0              | -1.285776               | -2.943544 | -0.047088 |
| 14               | 9                | 0              | -1.473682               | -3.906213 | 0.856020  |
| 15               | 9                | 0              | 0.023439                | -2.736805 | -0.179578 |
| 16               | 9                | 0              | -1.739494               | -3.396928 | -1.226269 |
| 17               | 9                | 0              | -1.689681               | -0.714362 | -0.605849 |
| 18               | 6                | 0              | -0.494254               | 1.748839  | 3.015174  |
| 19               | 1                | 0              | -0.190204               | 2.179134  | 3.973231  |
| 20               | 1                | 0              | 0.365867                | 1.239628  | 2.576427  |
| 21               | 1                | 0              | -0.786212               | 2.562339  | 2.347678  |
| 22               | 6                | 0              | -3.426431               | 2.128307  | 1.136056  |
| 23               | 1                | 0              | -3.188347               | 2.760294  | 1.994735  |
| 24               | 1                | 0              | -2.688936               | 2.316860  | 0.352961  |
| 25               | 1                | 0              | -4.411885               | 2.424087  | 0.769170  |

**1Bc\_CHCl<sub>3</sub>\_ωB97X-D/6-311++G(d,p)  $E = -927.2010494$** 

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -2.614053               | -0.850000 | 0.363280  |
| 2                | 1                | 0              | -2.215775               | -1.465484 | 1.169609  |
| 3                | 1                | 0              | -3.314630               | -0.148850 | 0.827281  |
| 4                | 6                | 0              | -1.889256               | 1.199769  | -0.826053 |
| 5                | 1                | 0              | -1.130639               | 1.515360  | -1.545332 |
| 6                | 1                | 0              | -2.792768               | 1.016661  | -1.411912 |
| 7                | 6                | 0              | -0.264090               | -0.264421 | 0.319571  |
| 8                | 9                | 0              | 0.011202                | -1.602970 | 0.428505  |
| 9                | 9                | 0              | -0.185815               | 0.189163  | 1.637091  |
| 10               | 7                | 0              | -1.511695               | -0.098166 | -0.258658 |
| 11               | 6                | 0              | 0.896640                | 0.395158  | -0.460209 |
| 12               | 1                | 0              | 0.719482                | 0.283516  | -1.531622 |
| 13               | 6                | 0              | 2.283369                | -0.207106 | -0.175572 |
| 14               | 9                | 0              | 2.401994                | -1.412659 | -0.738871 |
| 15               | 9                | 0              | 2.556643                | -0.321355 | 1.123756  |
| 16               | 9                | 0              | 3.218014                | 0.584261  | -0.717681 |
| 17               | 9                | 0              | 0.962280                | 1.731085  | -0.153004 |
| 18               | 6                | 0              | -2.144831               | 2.313692  | 0.187842  |
| 19               | 1                | 0              | -2.490157               | 3.209226  | -0.334565 |
| 20               | 1                | 0              | -2.914916               | 2.028891  | 0.908342  |
| 21               | 1                | 0              | -1.237361               | 2.565945  | 0.737163  |
| 22               | 6                | 0              | -3.332297               | -1.729187 | -0.650822 |
| 23               | 1                | 0              | -3.729551               | -1.137525 | -1.479640 |
| 24               | 1                | 0              | -2.648358               | -2.476317 | -1.058921 |
| 25               | 1                | 0              | -4.170317               | -2.245203 | -0.175306 |

**1Ca\_CHCl<sub>3</sub>\_ωB97X-D/6-311++G(d,p)  $E = -927.1969183$** 

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -1.650172               | -1.371434 | -0.847185 |
| 2                | 1                | 0              | -2.678239               | -1.236233 | -1.199539 |
| 3                | 1                | 0              | -1.015382               | -1.367901 | -1.731535 |
| 4                | 6                | 0              | -2.417950               | 0.289683  | 0.805356  |
| 5                | 1                | 0              | -3.058460               | 0.936160  | 0.188740  |
| 6                | 1                | 0              | -3.024023               | -0.582746 | 1.054956  |
| 7                | 6                | 0              | -0.278640               | 0.636649  | -0.386862 |
| 8                | 9                | 0              | 0.642290                | -0.032756 | -1.125931 |
| 9                | 9                | 0              | 0.407720                | 1.108904  | 0.710704  |
| 10               | 7                | 0              | -1.292749               | -0.239573 | 0.022281  |
| 11               | 6                | 0              | -0.679590               | 1.921473  | -1.154815 |
| 12               | 1                | 0              | -1.341377               | 2.516162  | -0.520502 |
| 13               | 6                | 0              | -1.403360               | 1.699192  | -2.487831 |
| 14               | 9                | 0              | -2.606478               | 1.144088  | -2.286838 |
| 15               | 9                | 0              | -0.725833               | 0.916423  | -3.328917 |
| 16               | 9                | 0              | -1.598152               | 2.874260  | -3.094562 |
| 17               | 9                | 0              | 0.446054                | 2.660221  | -1.425221 |
| 18               | 6                | 0              | -2.049912               | 0.996292  | 2.103457  |
| 19               | 1                | 0              | -2.967116               | 1.195165  | 2.662761  |
| 20               | 1                | 0              | -1.397622               | 0.368834  | 2.713462  |
| 21               | 1                | 0              | -1.546494               | 1.950184  | 1.939970  |
| 22               | 6                | 0              | -1.507636               | -2.701703 | -0.120393 |
| 23               | 1                | 0              | -0.468950               | -2.864526 | 0.174284  |
| 24               | 1                | 0              | -2.127692               | -2.729468 | 0.779702  |
| 25               | 1                | 0              | -1.820795               | -3.522914 | -0.770534 |

**1Cb\_CHCl<sub>3</sub>\_ωB97X-D/6-311++G(d,p)  $E = -927.1965531$** 

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 7                | 0              | -1.796147               | 2.212319  | 1.736062  |
| 2                | 6                | 0              | -1.206727               | 3.191993  | 2.668353  |
| 3                | 1                | 0              | -0.686991               | 2.690952  | 3.488744  |
| 4                | 1                | 0              | -2.040338               | 3.729548  | 3.121591  |
| 5                | 6                | 0              | -0.286684               | 4.180891  | 1.967688  |
| 6                | 1                | 0              | 0.095626                | 4.915003  | 2.681959  |
| 7                | 1                | 0              | -0.830250               | 4.711076  | 1.181738  |
| 8                | 1                | 0              | 0.566978                | 3.672506  | 1.514427  |
| 9                | 6                | 0              | -3.957962               | 3.331989  | 1.249894  |
| 10               | 1                | 0              | -3.678210               | 3.491246  | 0.207708  |
| 11               | 1                | 0              | -3.708979               | 4.234523  | 1.813200  |
| 12               | 1                | 0              | -5.040873               | 3.197175  | 1.304500  |
| 13               | 6                | 0              | -3.261014               | 2.102776  | 1.814188  |
| 14               | 1                | 0              | -3.583534               | 1.220889  | 1.263736  |
| 15               | 1                | 0              | -3.563735               | 1.936606  | 2.856149  |
| 16               | 6                | 0              | -1.094132               | 1.011443  | 1.540176  |
| 17               | 9                | 0              | 0.172021                | 1.123877  | 2.030223  |
| 18               | 9                | 0              | -1.649354               | -0.057411 | 2.216782  |
| 19               | 6                | 0              | -0.874034               | 0.584330  | 0.067338  |
| 20               | 1                | 0              | -0.246104               | 1.350630  | -0.392952 |
| 21               | 6                | 0              | -2.093038               | 0.391583  | -0.840975 |
| 22               | 9                | 0              | -1.692581               | -0.116935 | -2.011148 |
| 23               | 9                | 0              | -2.999637               | -0.447047 | -0.329067 |
| 24               | 9                | 0              | -2.698672               | 1.555677  | -1.095719 |
| 25               | 9                | 0              | -0.193608               | -0.610241 | 0.062852  |

**1Cc\_CHCl<sub>3</sub>\_ωB97X-D/6-311++G(d,p)  $E = -927.2022971$** 

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 2.391032                | -0.639352 | 0.458021  |
| 2                | 1                | 0              | 2.348525                | -1.730108 | 0.460845  |
| 3                | 1                | 0              | 3.263727                | -0.371944 | -0.143153 |
| 4                | 6                | 0              | 1.490353                | 0.810696  | -1.337798 |
| 5                | 1                | 0              | 2.124400                | 0.296142  | -2.071884 |
| 6                | 1                | 0              | 0.561919                | 1.063781  | -1.849406 |
| 7                | 6                | 0              | 0.143883                | -0.981123 | -0.379874 |
| 8                | 9                | 0              | 0.023226                | -1.763634 | 0.722854  |
| 9                | 9                | 0              | 0.346700                | -1.895984 | -1.424001 |
| 10               | 7                | 0              | 1.196384                | -0.088989 | -0.214345 |
| 11               | 6                | 0              | -1.238921               | -0.356369 | -0.668905 |
| 12               | 1                | 0              | -1.257600               | 0.094594  | -1.661433 |
| 13               | 6                | 0              | -1.686532               | 0.715186  | 0.336921  |
| 14               | 9                | 0              | -1.014125               | 1.855888  | 0.142448  |
| 15               | 9                | 0              | -1.525300               | 0.349707  | 1.608083  |
| 16               | 9                | 0              | -2.985712               | 0.979752  | 0.152534  |
| 17               | 9                | 0              | -2.167479               | -1.365284 | -0.641157 |
| 18               | 6                | 0              | 2.155142                | 2.098427  | -0.874790 |
| 19               | 1                | 0              | 2.331990                | 2.748526  | -1.734587 |
| 20               | 1                | 0              | 1.518444                | 2.625199  | -0.162015 |
| 21               | 1                | 0              | 3.120510                | 1.907783  | -0.400505 |
| 22               | 6                | 0              | 2.541534                | -0.112836 | 1.877610  |
| 23               | 1                | 0              | 2.614207                | 0.977121  | 1.881283  |
| 24               | 1                | 0              | 1.681482                | -0.400370 | 2.485555  |
| 25               | 1                | 0              | 3.443989                | -0.522546 | 2.339257  |

**1Aa\_C<sub>5</sub>H<sub>5</sub>N\_ωB97X-D/6-311++G(d,p)  $E = -927.2008071$** 

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -1.401207               | -1.287122 | 0.531842  |
| 2                | 1                | 0              | -0.506354               | -1.895957 | 0.393632  |
| 3                | 1                | 0              | -1.521136               | -1.164132 | 1.611691  |
| 4                | 6                | 0              | -1.543877               | 1.194771  | 0.806851  |
| 5                | 1                | 0              | -0.971289               | 1.153921  | 1.743060  |
| 6                | 1                | 0              | -1.245892               | 2.104358  | 0.286315  |
| 7                | 6                | 0              | -0.203508               | 0.228870  | -0.997572 |
| 8                | 9                | 0              | -0.563171               | 1.245056  | -1.854989 |
| 9                | 9                | 0              | -0.092976               | -0.897519 | -1.756695 |
| 10               | 7                | 0              | -1.204694               | 0.050184  | -0.043331 |
| 11               | 6                | 0              | 1.254049                | 0.604954  | -0.590548 |
| 12               | 1                | 0              | 1.872616                | 0.615263  | -1.490247 |
| 13               | 6                | 0              | 1.922946                | -0.317942 | 0.430783  |
| 14               | 9                | 0              | 1.970584                | -1.578964 | -0.010262 |
| 15               | 9                | 0              | 1.291507                | -0.313127 | 1.609758  |
| 16               | 9                | 0              | 3.179739                | 0.085648  | 0.649494  |
| 17               | 9                | 0              | 1.251567                | 1.864274  | -0.037799 |
| 18               | 6                | 0              | -3.034187               | 1.257812  | 1.110499  |
| 19               | 1                | 0              | -3.248766               | 2.144160  | 1.712270  |
| 20               | 1                | 0              | -3.612417               | 1.314176  | 0.185360  |
| 21               | 1                | 0              | -3.369129               | 0.384111  | 1.674857  |
| 22               | 6                | 0              | -2.602702               | -2.014476 | -0.058777 |
| 23               | 1                | 0              | -3.520064               | -1.440495 | 0.087427  |
| 24               | 1                | 0              | -2.464095               | -2.172735 | -1.130152 |
| 25               | 1                | 0              | -2.725074               | -2.989495 | 0.421303  |

**1Ab\_C<sub>5</sub>H<sub>5</sub>N\_ωB97X-D/6-311++G(d,p)  $E = -927.2034849$** 

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 1.192164                | 1.017137  | 1.255393  |
| 2                | 1                | 0              | 0.189107                | 1.152336  | 1.653791  |
| 3                | 1                | 0              | 1.817895                | 0.663168  | 2.085249  |
| 4                | 6                | 0              | 2.486314                | -0.411565 | -0.303224 |
| 5                | 1                | 0              | 3.237341                | 0.031664  | 0.355068  |
| 6                | 1                | 0              | 2.603846                | -1.492984 | -0.208605 |
| 7                | 6                | 0              | 0.234768                | -1.025791 | 0.331206  |
| 8                | 9                | 0              | 0.485836                | -1.865302 | 1.426885  |
| 9                | 9                | 0              | 0.318419                | -1.861704 | -0.745577 |
| 10               | 7                | 0              | 1.157001                | -0.000149 | 0.193863  |
| 11               | 6                | 0              | -1.266623               | -0.672196 | 0.452680  |
| 12               | 1                | 0              | -1.812663               | -1.600457 | 0.273864  |
| 13               | 6                | 0              | -1.778445               | 0.364253  | -0.555823 |
| 14               | 9                | 0              | -1.417355               | 0.047232  | -1.800312 |
| 15               | 9                | 0              | -1.344253               | 1.598870  | -0.294693 |
| 16               | 9                | 0              | -3.118108               | 0.399357  | -0.513652 |
| 17               | 9                | 0              | -1.586706               | -0.220034 | 1.709139  |
| 18               | 6                | 0              | 2.720476                | 0.021863  | -1.742714 |
| 19               | 1                | 0              | 3.726342                | -0.261754 | -2.064059 |
| 20               | 1                | 0              | 1.997797                | -0.452312 | -2.409786 |
| 21               | 1                | 0              | 2.617595                | 1.104859  | -1.842022 |
| 22               | 6                | 0              | 1.706927                | 2.351821  | 0.737750  |
| 23               | 1                | 0              | 2.734116                | 2.277731  | 0.373087  |
| 24               | 1                | 0              | 1.077014                | 2.715924  | -0.075986 |
| 25               | 1                | 0              | 1.693909                | 3.086974  | 1.545522  |

**1Ac\_C<sub>5</sub>H<sub>5</sub>N\_ωB97X-D/6-311++G(d,p) E = -927.1970861**

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 2.592441                | -0.492956 | -0.117858 |
| 2                | 1                | 0              | 3.426018                | -0.013453 | 0.400115  |
| 3                | 1                | 0              | 2.667902                | -1.557191 | 0.102488  |
| 4                | 6                | 0              | 1.030090                | 1.418254  | 0.277958  |
| 5                | 1                | 0              | 0.796437                | 1.624507  | -0.772566 |
| 6                | 1                | 0              | 0.149047                | 1.666670  | 0.864620  |
| 7                | 6                | 0              | 0.363925                | -0.942593 | 0.671725  |
| 8                | 9                | 0              | 0.837207                | -1.942012 | 1.508673  |
| 9                | 9                | 0              | 0.021133                | -1.674996 | -0.477329 |
| 10               | 7                | 0              | 1.342261                | 0.001157  | 0.478637  |
| 11               | 6                | 0              | -0.989955               | -0.528603 | 1.279503  |
| 12               | 1                | 0              | -1.490870               | -1.467342 | 1.518234  |
| 13               | 6                | 0              | -1.976636               | 0.273211  | 0.378603  |
| 14               | 9                | 0              | -3.149345               | -0.372903 | 0.320367  |
| 15               | 9                | 0              | -1.551193               | 0.429913  | -0.876839 |
| 16               | 9                | 0              | -2.214695               | 1.486214  | 0.881404  |
| 17               | 9                | 0              | -0.788669               | 0.157147  | 2.448390  |
| 18               | 6                | 0              | 2.161638                | 2.322742  | 0.746556  |
| 19               | 1                | 0              | 1.838738                | 3.363160  | 0.670884  |
| 20               | 1                | 0              | 2.417831                | 2.113598  | 1.787750  |
| 21               | 1                | 0              | 3.060729                | 2.212834  | 0.136820  |
| 22               | 6                | 0              | 2.701654                | -0.263115 | -1.622375 |
| 23               | 1                | 0              | 1.865892                | -0.726498 | -2.150167 |
| 24               | 1                | 0              | 2.720403                | 0.801013  | -1.870696 |
| 25               | 1                | 0              | 3.630631                | -0.704684 | -1.990550 |

**1Ba\_C<sub>5</sub>H<sub>5</sub>N\_ωB97X-D/6-311++G(d,p) E = -927.2009036**

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 2.229412                | -0.674432 | -0.877258 |
| 2                | 1                | 0              | 1.731960                | -1.567686 | -1.248737 |
| 3                | 1                | 0              | 2.139615                | 0.091501  | -1.656219 |
| 4                | 6                | 0              | 2.036536                | 0.981942  | 0.982074  |
| 5                | 1                | 0              | 1.371426                | 1.218442  | 1.813466  |
| 6                | 1                | 0              | 3.006588                | 0.761538  | 1.434446  |
| 7                | 6                | 0              | 0.182941                | -0.526608 | 0.496618  |
| 8                | 9                | 0              | -0.138913               | -0.554714 | 1.832796  |
| 9                | 9                | 0              | -0.091476               | -1.766244 | 0.009791  |
| 10               | 7                | 0              | 1.549248                | -0.253731 | 0.353767  |
| 11               | 6                | 0              | -0.802014               | 0.485387  | -0.142226 |
| 12               | 1                | 0              | -0.687847               | 1.444932  | 0.366912  |
| 13               | 6                | 0              | -2.292914               | 0.126666  | -0.114567 |
| 14               | 9                | 0              | -2.727802               | -0.049256 | 1.135102  |
| 15               | 9                | 0              | -2.572370               | -0.974655 | -0.813872 |
| 16               | 9                | 0              | -3.000965               | 1.131155  | -0.653613 |
| 17               | 9                | 0              | -0.456265               | 0.638561  | -1.466132 |
| 18               | 6                | 0              | 2.172954                | 2.190710  | 0.057003  |
| 19               | 1                | 0              | 2.485350                | 3.056097  | 0.645767  |
| 20               | 1                | 0              | 2.927537                | 2.026103  | -0.715320 |
| 21               | 1                | 0              | 1.233763                | 2.442344  | -0.441189 |
| 22               | 6                | 0              | 3.696742                | -0.988624 | -0.620783 |
| 23               | 1                | 0              | 4.260116                | -0.101435 | -0.321128 |
| 24               | 1                | 0              | 3.798052                | -1.743560 | 0.162379  |
| 25               | 1                | 0              | 4.151160                | -1.373808 | -1.536326 |

**1Bb\_C<sub>5</sub>H<sub>5</sub>N\_ωB97X-D/6-311++G(d,p)  $E = -927.2024324$** 

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 1.887530                | 1.298183  | 0.748379  |
| 2                | 1                | 0              | 1.040302                | 1.982822  | 0.750046  |
| 3                | 1                | 0              | 2.186724                | 1.155002  | 1.795247  |
| 4                | 6                | 0              | 2.492564                | -1.050642 | 0.213828  |
| 5                | 1                | 0              | 3.284053                | -0.722829 | 0.892839  |
| 6                | 1                | 0              | 2.063910                | -1.949012 | 0.662299  |
| 7                | 6                | 0              | 0.174351                | -0.404695 | 0.380582  |
| 8                | 9                | 0              | -0.075540               | -0.819836 | 1.702354  |
| 9                | 9                | 0              | -0.068243               | -1.527433 | -0.356617 |
| 10               | 7                | 0              | 1.473126                | 0.016349  | 0.165459  |
| 11               | 6                | 0              | -0.913878               | 0.654623  | 0.096655  |
| 12               | 1                | 0              | -0.967110               | 1.350159  | 0.935232  |
| 13               | 6                | 0              | -2.327784               | 0.084901  | -0.104479 |
| 14               | 9                | 0              | -2.690865               | -0.713365 | 0.900017  |
| 15               | 9                | 0              | -2.447100               | -0.593177 | -1.246203 |
| 16               | 9                | 0              | -3.201750               | 1.101960  | -0.153554 |
| 17               | 9                | 0              | -0.609012               | 1.349644  | -1.046732 |
| 18               | 6                | 0              | 3.065397                | -1.373669 | -1.158570 |
| 19               | 1                | 0              | 3.830296                | -2.150191 | -1.072896 |
| 20               | 1                | 0              | 2.280464                | -1.734483 | -1.826151 |
| 21               | 1                | 0              | 3.520168                | -0.489857 | -1.610927 |
| 22               | 6                | 0              | 3.017641                | 1.944087  | -0.039304 |
| 23               | 1                | 0              | 3.924936                | 1.336120  | -0.023189 |
| 24               | 1                | 0              | 2.721807                | 2.098077  | -1.079374 |
| 25               | 1                | 0              | 3.260228                | 2.912887  | 0.402734  |

**1Bc\_C<sub>5</sub>H<sub>5</sub>N\_ωB97X-D/6-311++G(d,p)  $E = -927.2025127$** 

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -2.641554               | -0.425119 | 0.681603  |
| 2                | 1                | 0              | -2.277538               | -1.302647 | 1.215344  |
| 3                | 1                | 0              | -3.139156               | 0.205030  | 1.424879  |
| 4                | 6                | 0              | -1.689244               | 1.744570  | -0.051981 |
| 5                | 1                | 0              | -0.953828               | 2.128778  | -0.761544 |
| 6                | 1                | 0              | -2.658473               | 1.861148  | -0.541553 |
| 7                | 6                | 0              | -0.243534               | -0.194649 | 0.439667  |
| 8                | 9                | 0              | -0.194973               | -1.536135 | 0.154875  |
| 9                | 9                | 0              | 0.045545                | -0.149522 | 1.807545  |
| 10               | 7                | 0              | -1.493152               | 0.300859  | 0.114088  |
| 11               | 6                | 0              | 0.932359                | 0.487866  | -0.296133 |
| 12               | 1                | 0              | 0.637047                | 0.712402  | -1.322643 |
| 13               | 6                | 0              | 2.213842                | -0.359740 | -0.377585 |
| 14               | 9                | 0              | 2.067497                | -1.360271 | -1.250491 |
| 15               | 9                | 0              | 2.585788                | -0.876494 | 0.794589  |
| 16               | 9                | 0              | 3.217472                | 0.411976  | -0.813824 |
| 17               | 9                | 0              | 1.261787                | 1.657407  | 0.343216  |
| 18               | 6                | 0              | -1.655666               | 2.567953  | 1.234390  |
| 19               | 1                | 0              | -1.858873               | 3.615734  | 1.000313  |
| 20               | 1                | 0              | -2.413318               | 2.232042  | 1.946044  |
| 21               | 1                | 0              | -0.679934               | 2.508247  | 1.717768  |
| 22               | 6                | 0              | -3.624837               | -0.850809 | -0.399478 |
| 23               | 1                | 0              | -3.998906               | 0.010489  | -0.958822 |
| 24               | 1                | 0              | -3.147609               | -1.536954 | -1.102429 |
| 25               | 1                | 0              | -4.483134               | -1.354619 | 0.052077  |

**1Ca\_C<sub>5</sub>H<sub>5</sub>N\_ωB97X-D/6-311++G(d,p)  $E = -927.1984853$** 

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | -1.671164               | -1.374340 | -0.841449 |
| 2                | 1                | 0              | -2.714142               | -1.248381 | -1.148849 |
| 3                | 1                | 0              | -1.075029               | -1.346490 | -1.752310 |
| 4                | 6                | 0              | -2.428555               | 0.288823  | 0.812003  |
| 5                | 1                | 0              | -3.076213               | 0.914932  | 0.182421  |
| 6                | 1                | 0              | -3.024384               | -0.583543 | 1.085706  |
| 7                | 6                | 0              | -0.283974               | 0.619691  | -0.377319 |
| 8                | 9                | 0              | 0.630520                | -0.056843 | -1.120003 |
| 9                | 9                | 0              | 0.412144                | 1.083803  | 0.719863  |
| 10               | 7                | 0              | -1.302606               | -0.248530 | 0.033310  |
| 11               | 6                | 0              | -0.674090               | 1.910271  | -1.140670 |
| 12               | 1                | 0              | -1.330704               | 2.508346  | -0.504926 |
| 13               | 6                | 0              | -1.394613               | 1.700332  | -2.477144 |
| 14               | 9                | 0              | -2.597151               | 1.143016  | -2.286884 |
| 15               | 9                | 0              | -0.711543               | 0.925520  | -3.322721 |
| 16               | 9                | 0              | -1.585372               | 2.880764  | -3.075236 |
| 17               | 9                | 0              | 0.459940                | 2.640526  | -1.406976 |
| 18               | 6                | 0              | -2.061735               | 1.030841  | 2.089919  |
| 19               | 1                | 0              | -2.981398               | 1.244390  | 2.639454  |
| 20               | 1                | 0              | -1.411671               | 0.421733  | 2.720568  |
| 21               | 1                | 0              | -1.561204               | 1.981458  | 1.900223  |
| 22               | 6                | 0              | -1.479954               | -2.713576 | -0.143819 |
| 23               | 1                | 0              | -0.425732               | -2.874275 | 0.091912  |
| 24               | 1                | 0              | -2.050613               | -2.757227 | 0.787672  |
| 25               | 1                | 0              | -1.821314               | -3.526802 | -0.789737 |

**1Cb\_C<sub>5</sub>H<sub>5</sub>N\_ωB97X-D/6-311++G(d,p)  $E = -927.1977361$** 

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 7                | 0              | -1.796715               | 2.212564  | 1.737631  |
| 2                | 6                | 0              | -1.210213               | 3.192702  | 2.672097  |
| 3                | 1                | 0              | -0.691496               | 2.691365  | 3.492804  |
| 4                | 1                | 0              | -2.045407               | 3.728265  | 3.124469  |
| 5                | 6                | 0              | -0.290395               | 4.183291  | 1.973725  |
| 6                | 1                | 0              | 0.091032                | 4.915544  | 2.690318  |
| 7                | 1                | 0              | -0.834245               | 4.715626  | 1.189422  |
| 8                | 1                | 0              | 0.563233                | 3.676358  | 1.518688  |
| 9                | 6                | 0              | -3.954323               | 3.335437  | 1.238925  |
| 10               | 1                | 0              | -3.670100               | 3.493040  | 0.197612  |
| 11               | 1                | 0              | -3.705616               | 4.237750  | 1.802539  |
| 12               | 1                | 0              | -5.037612               | 3.202400  | 1.289472  |
| 13               | 6                | 0              | -3.262522               | 2.105590  | 1.807898  |
| 14               | 1                | 0              | -3.583989               | 1.223555  | 1.257101  |
| 15               | 1                | 0              | -3.570335               | 1.942043  | 2.848581  |
| 16               | 6                | 0              | -1.095147               | 1.013450  | 1.542187  |
| 17               | 9                | 0              | 0.170113                | 1.123161  | 2.035507  |
| 18               | 9                | 0              | -1.651691               | -0.058389 | 2.218945  |
| 19               | 6                | 0              | -0.872149               | 0.583227  | 0.070696  |
| 20               | 1                | 0              | -0.241639               | 1.346303  | -0.390803 |
| 21               | 6                | 0              | -2.088896               | 0.386904  | -0.839552 |
| 22               | 9                | 0              | -1.685860               | -0.127173 | -2.006783 |
| 23               | 9                | 0              | -2.995605               | -0.451989 | -0.326134 |
| 24               | 9                | 0              | -2.695417               | 1.548198  | -1.099997 |
| 25               | 9                | 0              | -0.192984               | -0.613824 | 0.072098  |

**1Cc\_C<sub>5</sub>H<sub>5</sub>N\_ωB97X-D/6-311++G(d,p) E = -927.2037732**

Standard orientation:

| Center<br>Number | Atomic<br>Number | Atomic<br>Type | Coordinates (Angstroms) |           |           |
|------------------|------------------|----------------|-------------------------|-----------|-----------|
|                  |                  |                | X                       | Y         | Z         |
| 1                | 6                | 0              | 2.394110                | -0.618383 | 0.498283  |
| 2                | 1                | 0              | 2.341354                | -1.705907 | 0.575605  |
| 3                | 1                | 0              | 3.262776                | -0.400569 | -0.127720 |
| 4                | 6                | 0              | 1.492497                | 0.717889  | -1.383332 |
| 5                | 1                | 0              | 2.118200                | 0.148192  | -2.082519 |
| 6                | 1                | 0              | 0.563697                | 0.943722  | -1.906429 |
| 7                | 6                | 0              | 0.138421                | -0.993740 | -0.298410 |
| 8                | 9                | 0              | 0.011515                | -1.693512 | 0.859738  |
| 9                | 9                | 0              | 0.331809                | -1.988702 | -1.271310 |
| 10               | 7                | 0              | 1.197758                | -0.102215 | -0.199168 |
| 11               | 6                | 0              | -1.239998               | -0.382828 | -0.633723 |
| 12               | 1                | 0              | -1.258307               | -0.010169 | -1.658012 |
| 13               | 6                | 0              | -1.677562               | 0.764539  | 0.289348  |
| 14               | 9                | 0              | -0.996791               | 1.881952  | 0.014073  |
| 15               | 9                | 0              | -1.518216               | 0.490028  | 1.584834  |
| 16               | 9                | 0              | -2.975383               | 1.024497  | 0.088413  |
| 17               | 9                | 0              | -2.175801               | -1.381144 | -0.525091 |
| 18               | 6                | 0              | 2.172138                | 2.026957  | -1.011521 |
| 19               | 1                | 0              | 2.353143                | 2.612534  | -1.915546 |
| 20               | 1                | 0              | 1.542841                | 2.609413  | -0.336289 |
| 21               | 1                | 0              | 3.136507                | 1.858428  | -0.527150 |
| 22               | 6                | 0              | 2.565146                | 0.001161  | 1.877382  |
| 23               | 1                | 0              | 2.646642                | 1.088167  | 1.805556  |
| 24               | 1                | 0              | 1.711194                | -0.238232 | 2.514260  |
| 25               | 1                | 0              | 3.470624                | -0.383986 | 2.353777  |



**Table S1.** Calculated [ $\omega$ B97X-D/6-311++g(d,p)] spin-spin coupling constants and F–C–C–F dihedral angles, in implicit cyclohexane solvent.

| Conformer  | $^1J_{\text{C,Fpro-S}}$ | $^1J_{\text{C,Fpro-R}}$ | $^3J_{\text{F-2,Fpro-S}}$ | $^3J_{\text{F-2,Fpro-R}}$ | F-C-C-F(pro-S) | F-C-C-F(pro-R) |
|------------|-------------------------|-------------------------|---------------------------|---------------------------|----------------|----------------|
| <b>1Aa</b> | -260.7                  | -253.1                  | -20.2                     | -14.09                    | 57.0           | 169.2          |
| <b>1Ab</b> | -283.3                  | -235.3                  | -21.5                     | -14.69                    | 49.4           | 159.5          |
| <b>1Ac</b> | -229.9                  | -251.2                  | -17.4                     | -23.22                    | 70.4           | 177.5          |
| <b>1Ba</b> | -250.0                  | -262.8                  | -27.1                     | -14.89                    | 173.4          | -72.2          |
| <b>1Bb</b> | -265.2                  | -247.1                  | -30.2                     | -11.43                    | 163.0          | -85.5          |
| <b>1Bc</b> | -236.3                  | -280.2                  | -16.7                     | -27.84                    | 153.6          | -45.0          |
| <b>1Ca</b> | -259.4                  | -280.9                  | -9.7                      | -17.18                    | -46.8          | 64.5           |
| <b>1Cb</b> | -298.7                  | -260.1                  | -25.3                     | -17.8                     | -51.2          | 60.2           |
| <b>1Cc</b> | -249.8                  | -279.7                  | -8.2                      | -16.75                    | -48.0          | 63.2           |

**Table S2.** Calculated [ $\omega$ B97X-D/6-311++g(d,p)] spin-spin coupling constants and F–C–C–F dihedral angles, in implicit pyridine solvent.

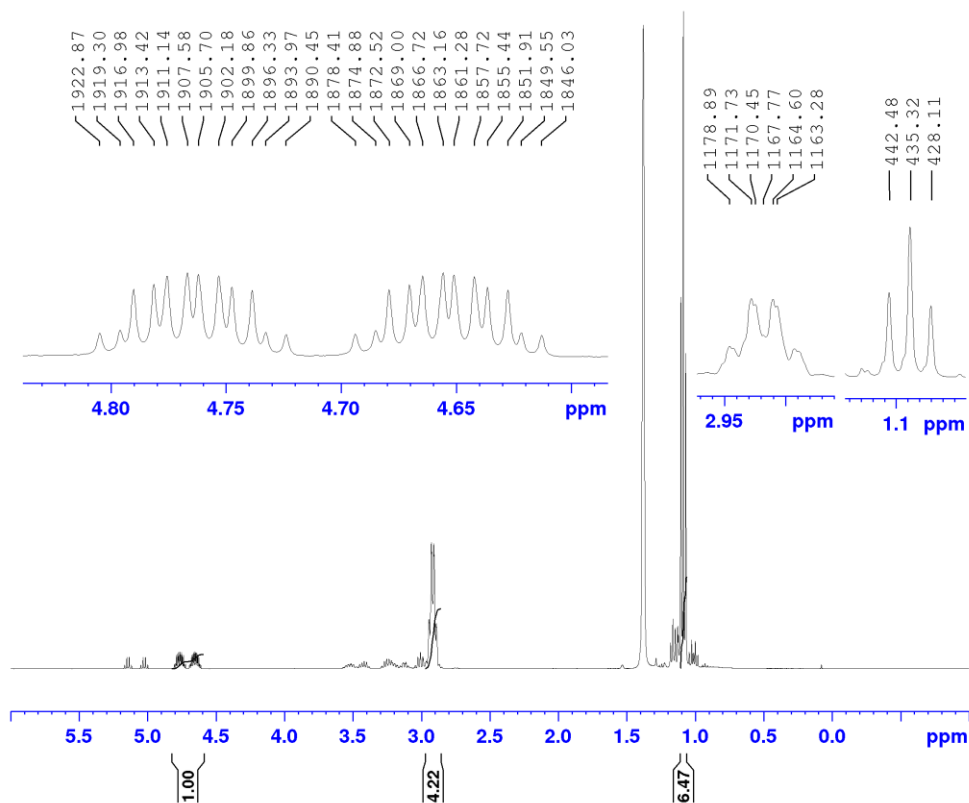
| Conformer  | $^1J_{\text{C,Fpro-S}}$ | $^1J_{\text{C,Fpro-R}}$ | $^3J_{\text{F-2,Fpro-S}}$ | $^3J_{\text{F-2,Fpro-R}}$ | F-C-C-F(pro-S) | F-C-C-F(pro-R) |
|------------|-------------------------|-------------------------|---------------------------|---------------------------|----------------|----------------|
| <b>1Aa</b> | -258.0                  | -252.7                  | -20.4                     | -13.1                     | 57.1           | 168.8          |
| <b>1Ab</b> | -281.2                  | -234.4                  | -22.1                     | -14.3                     | 50.7           | 159.7          |
| <b>1Ac</b> | -225.8                  | -252.8                  | -16.8                     | -24.1                     | 71.3           | 177.7          |
| <b>1Ba</b> | -248.7                  | -260.3                  | -25.7                     | -15.4                     | 175.2          | -71.2          |
| <b>1Bb</b> | -264.8                  | -243.1                  | -30.1                     | -12.1                     | 166.8          | -82.8          |
| <b>1Bc</b> | -231.9                  | -275.8                  | -18.0                     | -30.3                     | 155.8          | -45.4          |
| <b>1Ca</b> | -258.4                  | -255.1                  | -22.3                     | -31.7                     | -56.0          | 55.5           |
| <b>1Cb</b> | -296.6                  | -259.9                  | -27.3                     | -18.2                     | -50.8          | 60.1           |
| <b>1Cc</b> | -245.7                  | -278.5                  | -8.3                      | -17.1                     | -48.7          | 61.3           |

**Table S3.** Calculated  $^3J_{\text{H}_2,\text{F}1}$  coupling constants (in Hz) and H–C–C–F(1) dihedral angles (in degrees) for the optimized geometries of **1**, in cyclohexane and pyridine implicit solvents.

| Conf.      | Cyclohexane             |                         |                          |                          | Pyridine                |                         |                          |                          |
|------------|-------------------------|-------------------------|--------------------------|--------------------------|-------------------------|-------------------------|--------------------------|--------------------------|
|            | $^3J_{\text{H,Fpro-R}}$ | $^3J_{\text{H,Fpro-S}}$ | H-C-C-F <sub>pro-R</sub> | H-C-C-F <sub>pro-S</sub> | $^3J_{\text{H,Fpro-R}}$ | $^3J_{\text{H,Fpro-S}}$ | H-C-C-F <sub>pro-R</sub> | H-C-C-F <sub>pro-S</sub> |
| <b>1Aa</b> | -0.1                    | -1.5                    | 50.9                     | -61.3                    | -0.2                    | -1.5                    | 50.4                     | -61.2                    |
| <b>1Ab</b> | 9.9                     | -0.3                    | 41.3                     | -68.9                    | 9.9                     | -0.3                    | 41.8                     | -67.2                    |
| <b>1Ac</b> | 2.8                     | 9.9                     | 59.5                     | -48.7                    | 1.8                     | 10.8                    | 61.5                     | -44.9                    |
| <b>1Ba</b> | 15.6                    | 0.2                     | 169.6                    | 55.2                     | 15.9                    | -0.3                    | 171.0                    | 57.3                     |
| <b>1Bb</b> | 13.9                    | 1.0                     | 154.3                    | 42.9                     | 14.3                    | 0.5                     | 157.3                    | 46.9                     |
| <b>1Bc</b> | 8.3                     | -0.9                    | 164.6                    | 83.8                     | 8.6                     | -0.7                    | -165.1                   | 84.5                     |
| <b>1Ca</b> | 0.8                     | 9.8                     | -53.8                    | -165.0                   | 0.5                     | 14.0                    | -62.8                    | -174.3                   |
| <b>1Cb</b> | 6.8                     | 8.9                     | -56.9                    | -168.3                   | 6.8                     | 9.1                     | -57.0                    | -167.9                   |
| <b>1Cc</b> | 0.1                     | 9.3                     | -55.0                    | -166.2                   | -0.2                    | 9.5                     | -56.8                    | -166.8                   |

**Table S4.** Relative nuclear-electronic energies (in kcal mol<sup>-1</sup> and % population in parenthesis) and molecular dipole moments (in D) for the conformers of **1**, calculated at the MP2/6-311++g(d,p) level.

| Conf.      | Cyclohexane            |     | Chloroform             |     | Pyridine               |     |
|------------|------------------------|-----|------------------------|-----|------------------------|-----|
|            | G <sup>0</sup> rel (%) | μ   | G <sup>0</sup> rel (%) | μ   | G <sup>0</sup> rel (%) | μ   |
| <b>1Aa</b> | 2.3 (1)                | 1.5 | 2.3 (1)                | 1.6 | 2.4 (1)                | 1.7 |
| <b>1Ab</b> | 0.0 (65)               | 2.1 | 0.0 (49)               | 2.2 | 0.2 (37)               | 2.2 |
| <b>1Ac</b> | 5.9 (0)                | 2.4 | 5.8 (0)                | 2.5 | 5.9 (0)                | 2.6 |
| <b>1Ba</b> | 3.1 (0)                | 4.5 | 2.8 (0)                | 4.8 | 2.8 (0)                | 5.0 |
| <b>1Bb</b> | 1.6 (5)                | 4.5 | 1.2 (6)                | 4.8 | 1.1 (8)                | 5.0 |
| <b>1Bc</b> | 1.9 (3)                | 4.7 | 1.5 (4)                | 5.1 | 1.4 (4)                | 5.4 |
| <b>1Ca</b> | 4.7 (0)                | 4.4 | 4.3 (0)                | 4.8 | 4.2 (0)                | 5.1 |
| <b>1Cb</b> | 4.1 (0)                | 4.2 | 3.9 (0)                | 4.5 | 4.0 (0)                | 4.6 |
| <b>1Cc</b> | 0.6 (26)               | 4.5 | 0.1 (40)               | 4.9 | 0.0 (50)               | 5.2 |



## F2 - Acquisition Parameters

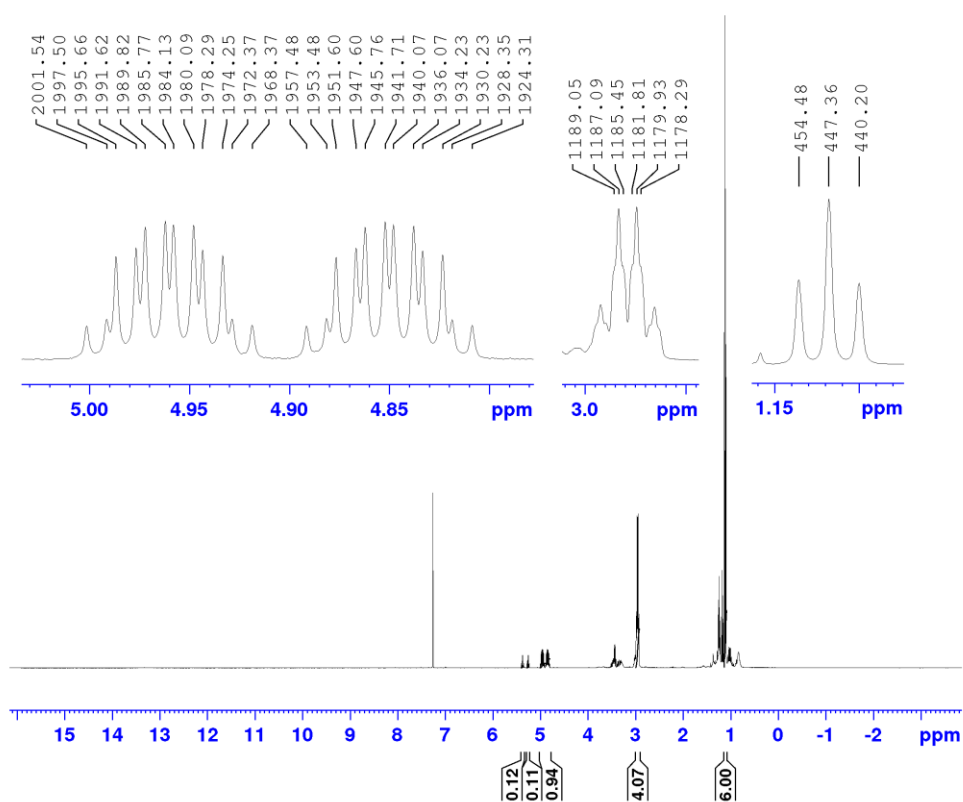
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 FIDRES 0.489064 Hz  
 AQ 2.0447233 sec  
 RG 203  
 DW 62.400 usec  
 DE 7.00 usec  
 TE 298.3 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 400.1824713 MHz  
 NUC1 1H  
 P1 8.50 usec  
 PLW1 11.30000019 W

## F2 - Processing parameters

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 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

**Figure S1.**  $^1\text{H}$  NMR spectrum of **1** in  $10 \text{ mg mL}^{-1}$  cyclohexane- $d_{12}$  solution.

CDC13 - 400 MHz - 1H

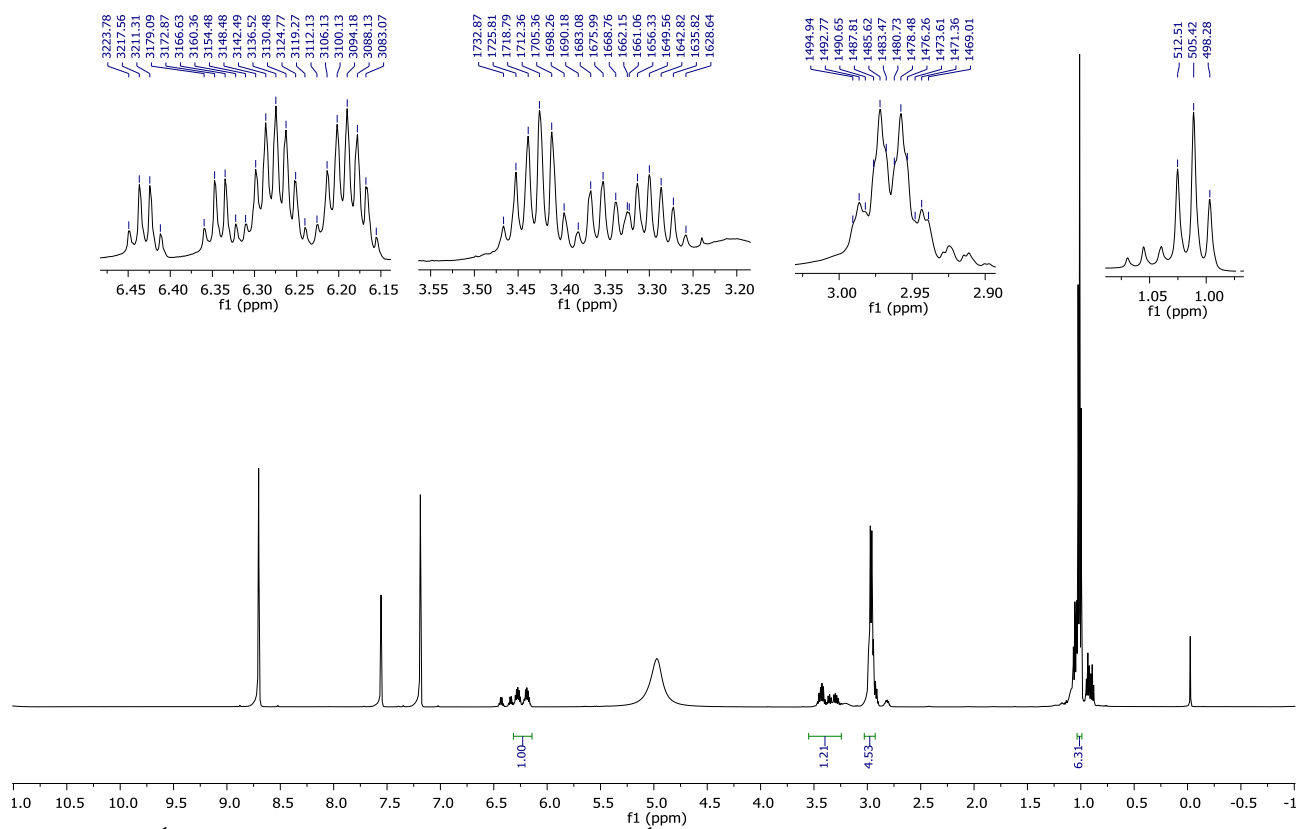


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FIDRES 0.489064 Hz  
AQ 2.0447233 sec  
RG 203  
DM 62.400 usec  
DE 7.00 usec  
TE 298.2 K  
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P1 8.50 usec  
PLW1 11.30000019 W

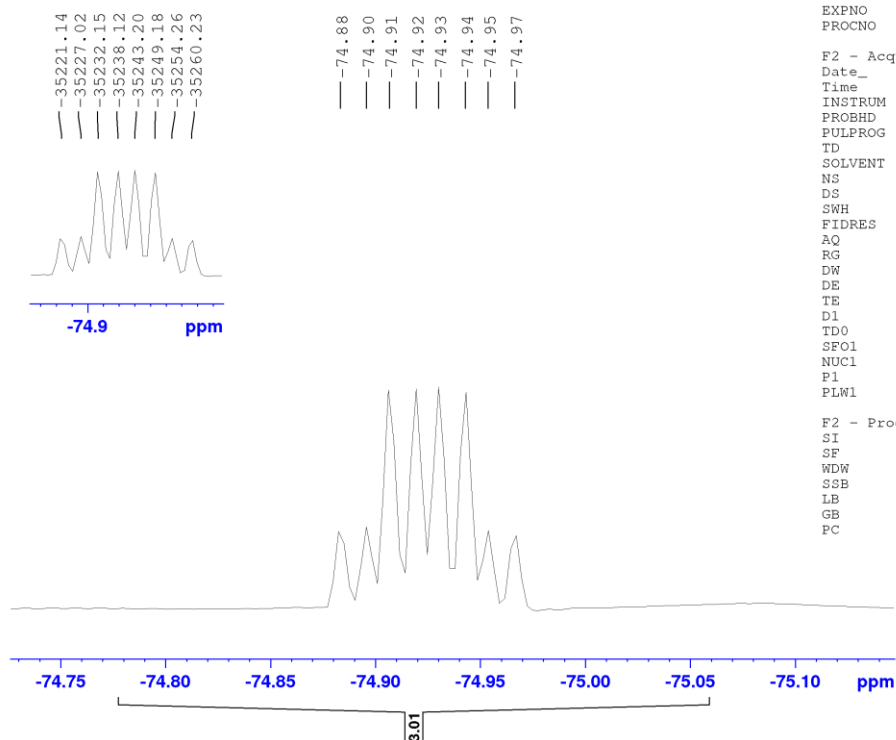
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LB 0.30 Hz  
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PC 1.00

**Figure S2.**  $^1\text{H}$  NMR spectrum of **1** in  $10\text{ mg mL}^{-1}$   $\text{CDCl}_3$  solution.



**Figure S3.**  $^1\text{H}$  NMR spectrum of **1** in  $10\text{ mg mL}^{-1}$  pyridine- $d_5$  solution.

Lucas - Ishikawa's Reagent  
 jan21luzH1 - C6D12 - 500 MHz - 19F-coupled



Current Data Parameters  
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 EXPNO 2  
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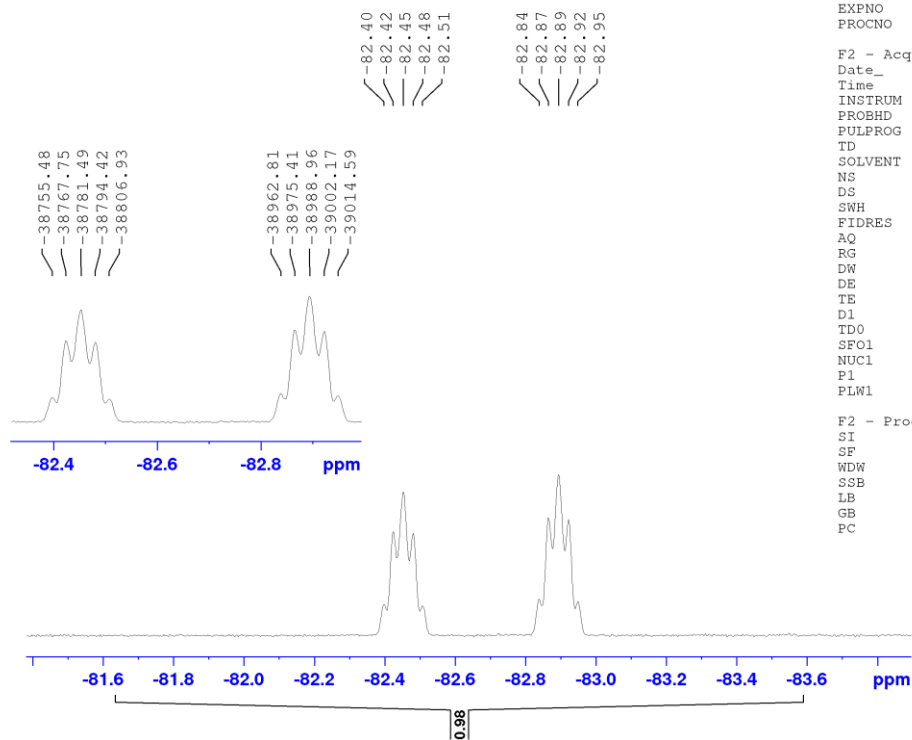
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 FIDRES 1.243923 Hz  
 AQ 0.8039083 sec  
 RG 287  
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 DE 10.00 usec  
 TE 300.2 K  
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 NUC1 19F  
 P1 16.60 usec  
 PLW1 54.00000000 W

F2 - Processing parameters  
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 LB -1.50 Hz  
 GB 0.2  
 PC 1.00

**Figure S4.**  $^{19}\text{F}$  NMR spectrum (expansion in the  $\text{CF}_3$  region) of **1** in  $10 \text{ mg mL}^{-1}$  cyclohexane- $d_{12}$  solution.



Lucas - Ishikawa's Reagent  
 jan21luzH1 - C6D12 - 500 MHz - 19F-coupled



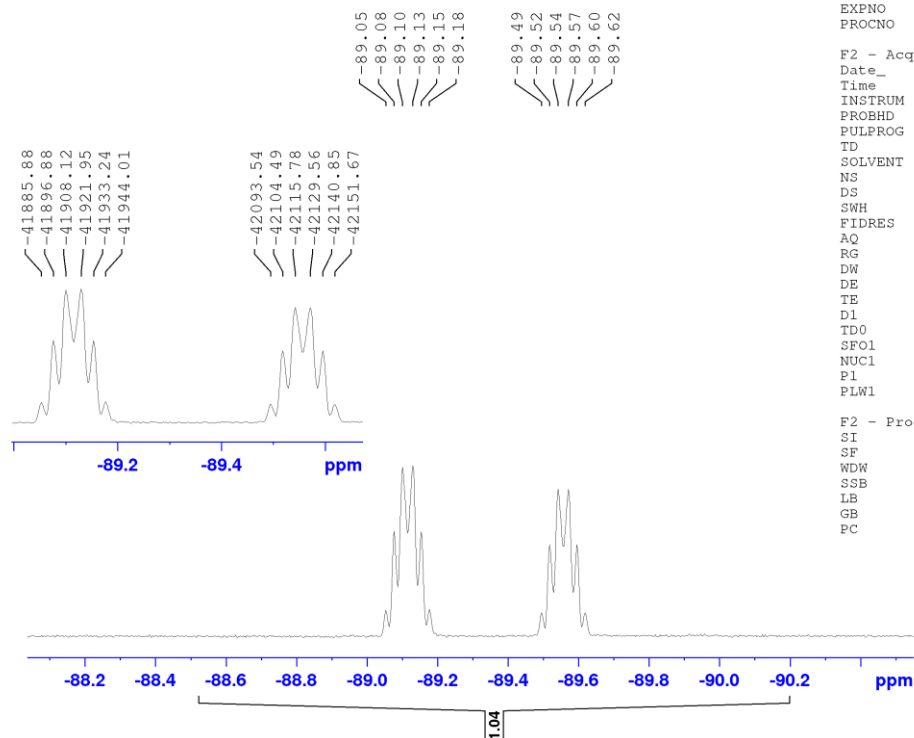
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 SOLVENT Acetone  
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 SWH 81521.742 Hz  
 FIDRES 1.243923 Hz  
 AQ 0.8039083 sec  
 RG 287  
 DW 6.133 usec  
 DE 10.00 usec  
 TE 300.2 K  
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 SFO1 470.2842360 MHz  
 NUC1 19F  
 P1 16.60 usec  
 PLW1 54.00000000 W

F2 - Processing parameters  
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 SF 470.3477330 MHz  
 WDW GM  
 SSB 0  
 LB -1.50 Hz  
 GB 0.2  
 PC 1.00

**Figure S5.**  $^{19}\text{F}$  NMR spectrum (expansion in the  $F_{\text{pro-S}}$  region) of **1** in 10 mg mL $^{-1}$  cyclohexane- $d_{12}$  solution.

Lucas - Ishikawa's Reagent  
 jan21luzH1 - C6D12 - 500 MHz - <sup>19</sup>F-coupled

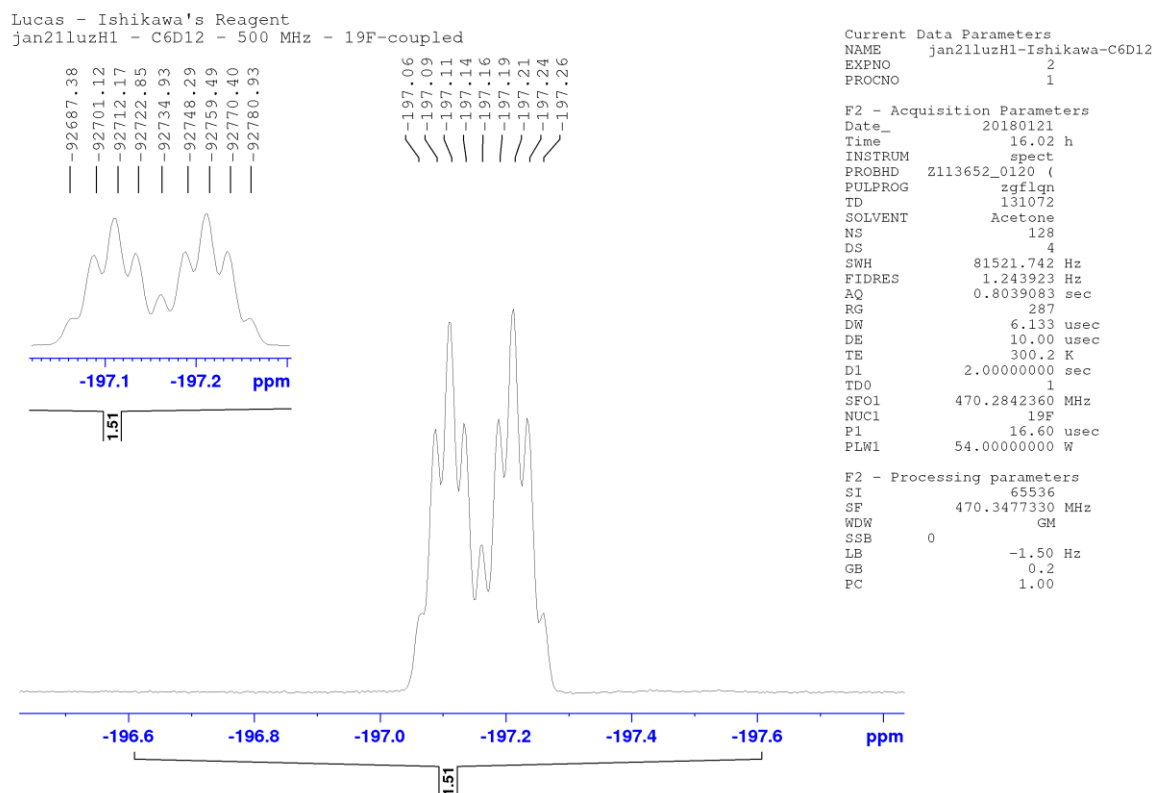


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 PROCNO 1

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 TD 131072  
 SOLVENT Acetone  
 NS 128  
 DS 4  
 SWH 81521.742 Hz  
 FIDRES 1.243923 Hz  
 AQ 0.8039083 sec  
 RG 287  
 DW 6.133 usec  
 DE 10.00 usec  
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 SFO1 470.2842360 MHz  
 NUC1 <sup>19</sup>F  
 P1 16.60 usec  
 PLW1 54.00000000 W

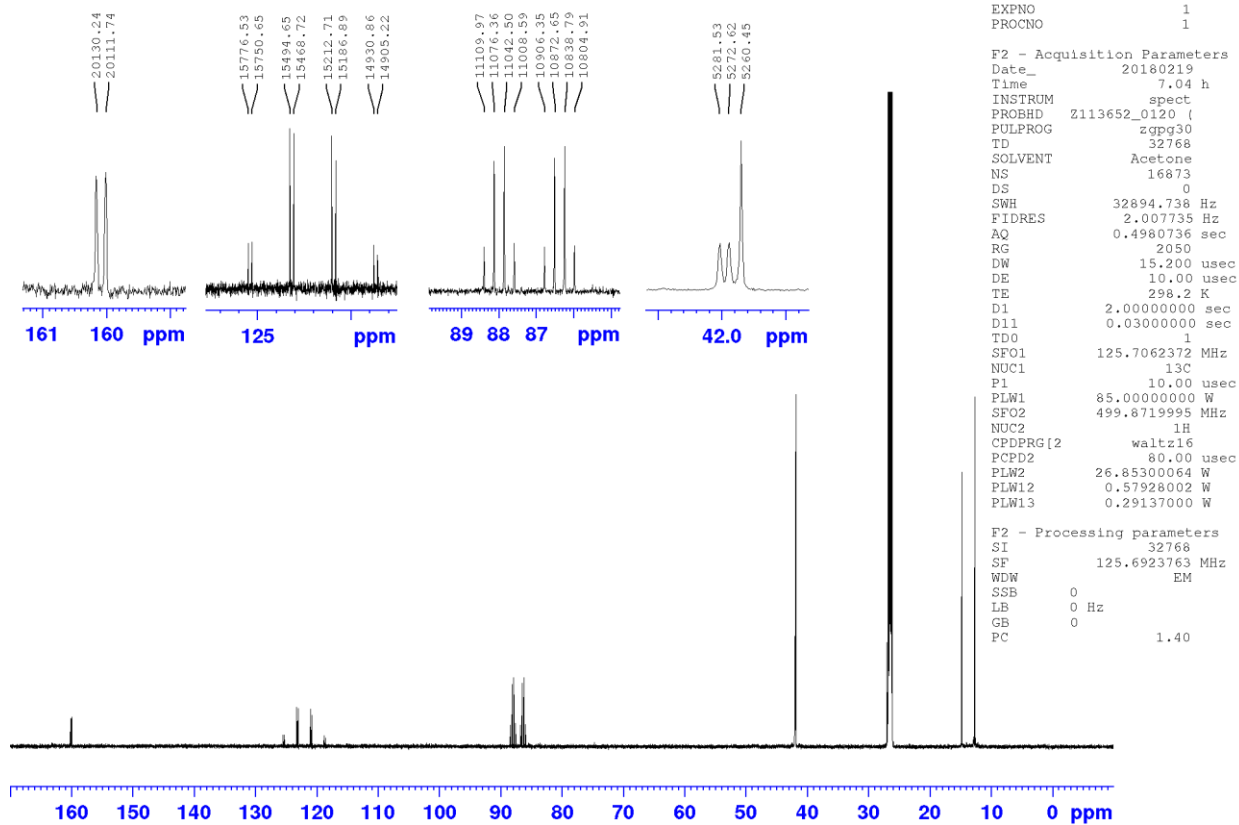
F2 - Processing parameters  
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 LB -1.50 Hz  
 GB 0.2  
 PC 1.00

**Figure S6.** <sup>19</sup>F NMR spectrum (expansion in the F<sub>pro-R</sub> region) of **1** in 10 mg mL<sup>-1</sup> cyclohexane-*d*<sub>12</sub> solution.

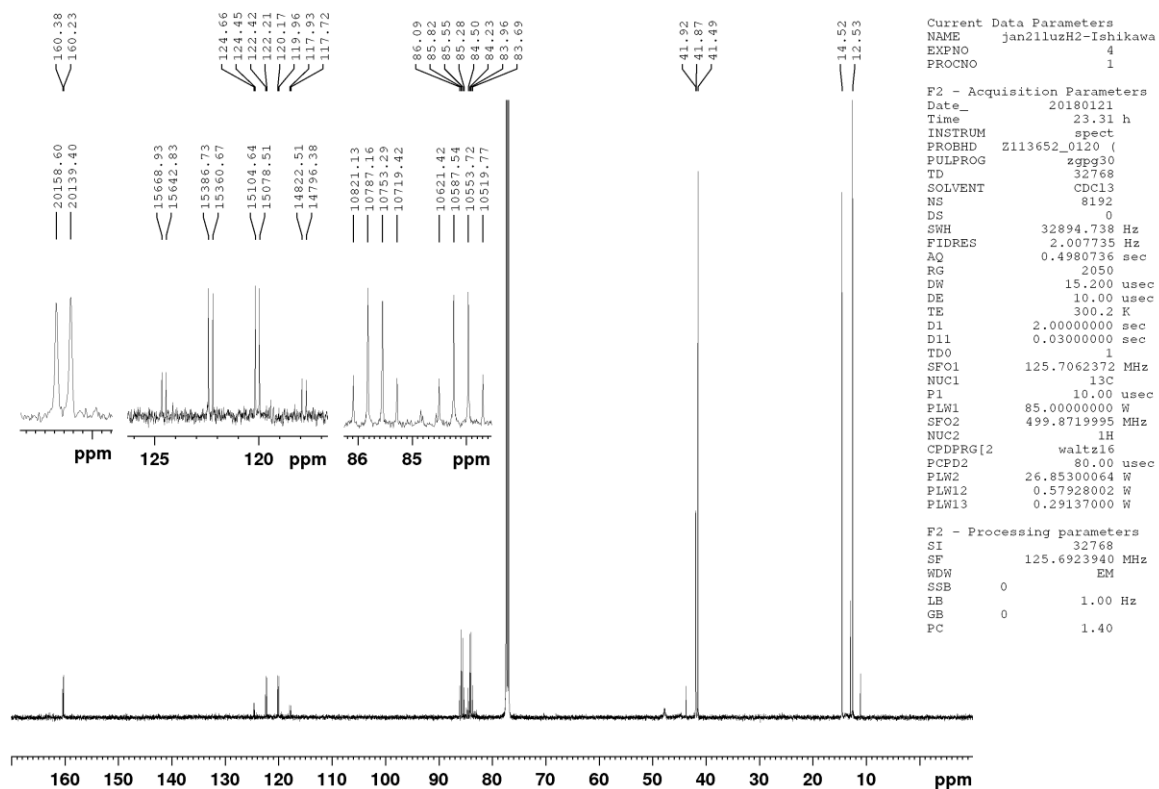


**Figure S7.**  $^{19}\text{F}$  NMR spectrum (expansion in the F-2 region) of **1** in  $10\text{ mg mL}^{-1}$  cyclohexane- $d_{12}$  solution.

Lucas - 13C - Ishikawa - C6D12  
500 MHz - fev16luzC1 - 13C{1H}

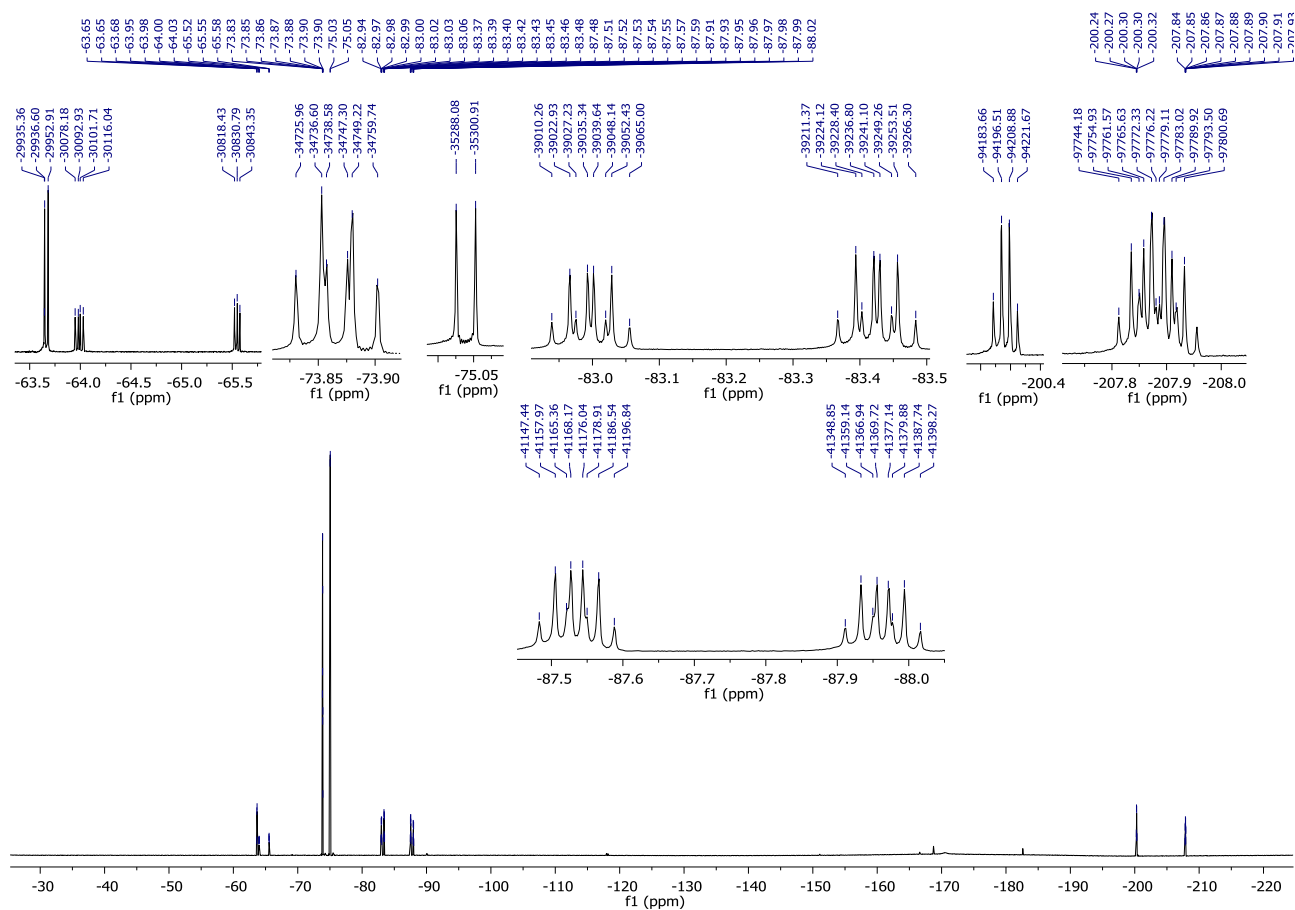


**Figure S8.**  $^{13}\text{C}$  NMR spectrum of **1** in 10 mg mL $^{-1}$  cyclohexane- $d_{12}$  solution.



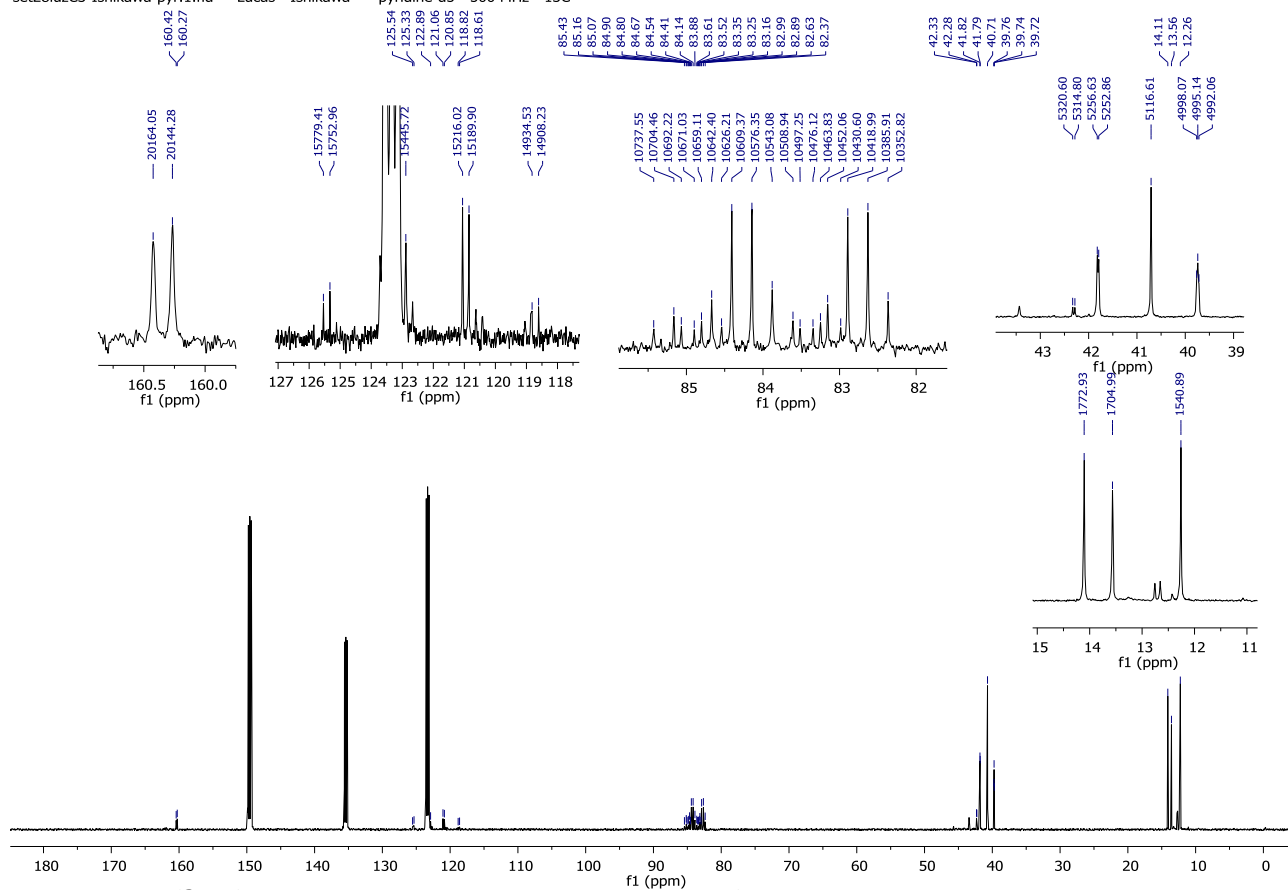
**Figure S9.**  $^{13}\text{C}$  NMR spectrum of **1** in 10 mg mL $^{-1}$  CDCl $_3$  solution.





**Figure S11.**  $^{19}\text{F}\{^1\text{H}\}$  NMR spectrum of **1** in  $10 \text{ mg mL}^{-1}$  pyridine- $d_5$  solution.

set28luzC3-Ishikawa-pyr.1.fid — Lucas - Ishikawa — pyridine-d5 - 500 MHz - 13C



**Figure S12.**  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **1** in  $10\text{ mg mL}^{-1}$  pyridine- $d_5$  solution.