Supporting Information (82 pages)

Importance of Solvent-Bridged Structures of Fluorinated Diphenylalanines. Synthesis, Detailed NMR Analysis, and Rotational Profiles of Phe(2-F)-Phe(2-F), Phe(2-F)-Phe, and Phe-Phe(2-F)

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Synthesis of mono1 F-FF and mono2 F-FF

Synthesis of mono1 F-FF: 1.2 g (3 mMol) of Fmoc-L-Phe(2-F)-OH were added to the resin together with 1.7 ml (10 mMol) of N,N-diisopropylethylamine (DIPEA). The reaction was left to proceed for 1 hour and then repeated. Capping of the resin was then performed with MeOH (5 min, 15 ml) and the loading of the resin was experimentally shown to be \( \approx 0.6 \text{ mMol/g} \) by HPLC based quantitative Fmoc evaluation test. Fmoc deprotection was achieved by treatment with 20% piperidine in DMF for 20 min, repeated twice.

2.4 g (6 mMol) of the second protected amino acid, Fmoc-L-Phe-OH was reacted with 3.4 ml of DIPEA (20 mMol) and subsequently with 2 g (5.5 mMol) of 2-(1H-benzotriazol-1-yl)-1,1,3,3-tetramethyluronium hexafluorophosphate (HBTU) for 5 min to provide the corresponding activated ester. This activated ester was reacted in situ with the peptydil resin for 1 hour. The same coupling procedure was repeated once to afford the protected dipeptide on the resin. Capping of unreacted amino groups of the first phenylalanine residue by acylation was achieved by reaction with 5% Ac\(_2\)O and DIPEA for 5 min. Final Fmoc deprotection was performed as above to obtain the desired dipeptide on the resin.

Acid-catalyzed ester hydrolysis was used to cleave the peptide from the resin and involved treatment with 10% trifluoroacetic acid (TFA) in presence of water and triisopropylsilane (TIPS) scavangers (both 5%) in dichloromethane (DCM). After 45 min of reaction, the reaction mixture was filtered and evaporated by nitrogen to almost dryness before to be diluted with 50% water and acetonitrile and lyophilized overnight to obtain 400 mg of crude dipeptide. Crude dipeptide identity was confirmed by LC-MS analysis and its preparative purification by MS-assisted flash chromatography yielded 240 mg of 95% pure H\(_2\)N-Phe(2-F)-Phe-COOH.

As this last contained however a small amount of a quite colorful contaminant, these were furtherly purified by MS assisted preparative HPLC to yield to obtain 130 mg of final purified colorless product.
**Synthesis of Mono2 F-FF:** 1.2 g (3 mMol) of Fmoc-L-Phe-OH were added to the resin together with 1.7 ml (10 mMol) of N,N-diisopropylethylamine (DIPEA). The reaction was left to proceed for 1 hour and then repeated. Capping of the resin was then performed with MeOH (5 min, 15 ml) and the loading of the resin was experimentally shown to be ≈ 0.6 mMol/g by HPLC based quantitative Fmoc evaluation test. Fmoc deprotection was achieved by treatment with 20% piperidine in DMF for 20 min, repeated twice.

2.4 g (6 mMol) of the second protected amino acid, Fmoc-L-Phe(2-F)-OH was reacted with 3.4 ml of DIPEA (20 mMol) and subsequently with 2 g (5.5 mMol) of 2-(1H-benzotriazol-1-yl)-1,1,3,3-tetramethyluronium hexafluorophosphate (HBTU) for 5 min to provide the corresponding activated ester. This activated ester was reacted in situ with the peptydil resin for 1 hour. The same coupling procedure was repeated once to afford the protected dipeptide on the resin. Capping of unreacted amino groups of the first phenylalanine residue by acylation was achieved by reaction with 5% Ac₂O and DIPEA for 5 min. Final Fmoc deprotection was performed as above to obtain the desired dipeptide on the resin.

Acid-catalyzed ester hydrolysis was used to cleave the peptide from the resin and involved treatment with 10% trifluoroacetic acid (TFA) in presence of water and triisopropylsilane (TIPS) scavengers (both 5%) in dichloromethane (DCM). After 45 min of reaction, the reaction mixture was filtered and evaporated by nitrogen to almost dryness before to be diluted with 50% water and acetonitrile and lyophilized overnight to obtain 350 mg of crude dipeptide. Crude dipeptide identity was confirmed by LC-MS analysis and its preparative purification by MS-assisted flash chromatography yielded 225 mg of 95% pure H₂N-Phe(2-F)-Phe-COOH.
**Figure S1.** GC chromatogram (top) and MS spectrum of di F-FF (bottom).
Figure S2. GC chromatogram (top) and MS spectrum of mono1 F-FF (bottom).
Figure S3. GC chromatogram (top) and MS spectrum of mono2 F-FF (bottom).
Experimental NMR Spectra of di F-FF

Figure S4. H-NMR spectrum of di F-FF.
Figure S5. C-NMR spectrum of di F-FF.
Figure S6a. F-NMR spectrum of di F-FF, decoupled.
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Experimental NMR Spectra of mono1 F-FF

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Figure S21. HMBC spectrum of mono2 F-FF.
# Potential Energy Surface Analysis

## Table S1. Energies and Thermochemistry of FF and Fluorinated Derivatives Computed at the SMD(B3LYP/6-31G*) Level

| Molecule | Total Energy [Hartree] | Vibrational Zero-Point Energy [kcal/mol] | Thermal Energy [kcal/mol] | Entropy $S_{\text{tot}}$ [cal/(mol-K)] | Translational Entropy $S_{\text{trans}}$ [cal/(mol-K)] | Lowest Vibr. Frequency [cm$^{-1}$] | Dipole Moment [Debye] |
|----------|------------------------|----------------------------------------|---------------------------|--------------------------------------|-------------------------------------------|---------------------------------|---------------------|
| water    | -76.422116             | 13.17                                  | 14.95                     | 45.16                                | 34.61                                     | 1677.32                        | 2.51                |
| **FF**   |                        |                                        |                           |                                      |                                           |                                 |                     |
| M1       | -1033.189202           | 224.89                                 | 237.98                    | 156.92                               | 43.11                                     | 18.47                          | 23.62               |
| M1-CIP   | -1033.188540           | 224.49                                 | 237.58                    | 159.31                               | 43.11                                     | 12.65                          | 17.41               |
| M1-N1    | -1033.185687           | 223.52                                 | 236.47                    | 156.12                               | 43.11                                     | 14.80                          | 10.36               |
| M1-N2    | -1033.190247           | 223.21                                 | 236.51                    | 159.00                               | 43.11                                     | 17.19                          | 6.27                |
| M1-N3    | -1033.188503           | 223.34                                 | 236.63                    | 159.97                               | 43.11                                     | 16.01                          | 5.67                |
| M3       | -1033.196290           | 224.71                                 | 237.93                    | 158.83                               | 43.11                                     | 18.43                          | 26.29               |
| M1a      | -1109.633799           | 240.19                                 | 254.79                    | 169.99                               | 43.28                                     | 9.22                           | 20.05               |
| M1b      | -1109.630305           | 240.35                                 | 255.15                    | 169.69                               | 43.28                                     | 19.00                          | 25.49               |
| **Mono1 F-FF** |                  |                                        |                           |                                      |                                           |                                 |                     |
| M1       | -1132.423262           | 219.58                                 | 233.26                    | 163.22                               | 43.28                                     | 13.05                          | 22.27               |
| M1-CIP   | -1132.422581           | 219.85                                 | 233.26                    | 159.43                               | 43.28                                     | 14.30                          | 17.33               |
| M1-N1    | -1132.419385           | 218.53                                 | 231.96                    | 159.10                               | 43.28                                     | 16.19                          | 8.81                |
| M1-N2    | -1132.423082           | 218.19                                 | 231.96                    | 161.46                               | 43.28                                     | 18.48                          | 5.61                |
| M1-N3    | -1132.421443           | 218.31                                 | 232.08                    | 162.32                               | 43.28                                     | 20.46                          | 6.12                |
| M3       | -1132.430725           | 219.43                                 | 233.00                    | 161.22                               | 43.28                                     | 17.11                          | 23.88               |
| M1a      | -1208.867628           | 235.07                                 | 250.19                    | 172.68                               | 43.44                                     | 14.59                          | 20.55               |
| M1b      | -1208.865849           | 235.28                                 | 250.55                    | 173.52                               | 43.44                                     | 16.03                          | 22.26               |
| M3b      | -1208.867027           | 235.28                                 | 250.51                    | 171.65                               | 43.44                                     | 20.59                          | 22.11               |
| **Mono2 F-FF** |                |                                        |                           |                                      |                                           |                                 |                     |
| M1       | -1132.424423           | 219.83                                 | 233.42                    | 159.20                               | 43.28                                     | 20.07                          | 23.48               |
| M1-CIP   | -1132.422366           | 219.86                                 | 233.32                    | 158.91                               | 43.28                                     | 17.64                          | 17.29               |
| M1-N1    | -1132.418981           | 218.35                                 | 231.81                    | 158.66                               | 43.28                                     | 18.56                          | 10.94               |
| M1-N2    | -1132.425944           | 218.19                                 | 231.95                    | 160.14                               | 43.28                                     | 22.47                          | 7.86                |
| M1-N3    | -1132.424277           | 218.31                                 | 232.05                    | 160.77                               | 43.28                                     | 21.04                          | 7.64                |
| M2       | -1132.428870           | 219.71                                 | 233.39                    | 161.81                               | 43.28                                     | 14.62                          | 26.25               |
| M3       | -1132.429441           | 219.49                                 | 233.29                    | 165.31                               | 43.28                                     | 12.40                          | 26.18               |
| M1a      | -1208.869801           | 235.14                                 | 250.19                    | 170.27                               | 43.44                                     | 16.17                          | 21.13               |
| M2b      | -1208.866864           | 235.59                                 | 250.71                    | 170.53                               | 43.44                                     | 17.73                          | 24.43               |
Table S2. Energies and Thermochemistry of FF and Fluorinated Derivatives Computed at the SMD(MP2/6-31G*) Level

| Molecule   | Total Energy [Hartree] | Vibrational Zero-Point Energy [kcal/mol] | Thermal Energy [kcal/mol] | Entropy S\textsubscript{tot} [cal/(mol·K)] | Translational Entropy S\textsubscript{trans} [cal/(mol·K)] | Lowest Vibr. Frequency [cm\textsuperscript{-1}] | Dipole Moment [Debye] |
|------------|------------------------|-----------------------------------------|---------------------------|------------------------------------------|--------------------------------------------------|-----------------------------------------------|----------------------|
| H\textsubscript{2}O | -76.211405              | 13.32                                   | 15.10                     | 45.16                                    | 34.61                                            | 1698.22                                       | 2.67                 |
| FF         |                        |                                         |                           |                                          |                                                  |                                               |                      |
| M1         | -1029.986718            | 226.01                                  | 239.30                    | 156.38                                   | 43.11                                            | 20.56                                         | 25.22                |
| M1a        | -1106.218673            | 241.85                                  | 256.54                    | 164.74                                   | 43.28                                            | 23.20                                         | 21.11                |
| Mono1 FF   |                        |                                         |                           |                                          |                                                  |                                               |                      |
| M1         | -1129.005608            | 221.26                                  | 234.93                    | 159.83                                   | 43.28                                            | 16.47                                         | 21.61                |
| M1a        | -1205.236987            | 236.64                                  | 251.91                    | 172.24                                   | 43.44                                            | 16.45                                         | 22.21                |
| Mono2 FF   |                        |                                         |                           |                                          |                                                  |                                               |                      |
| M1         | -1129.005701            | 221.19                                  | 234.82                    | 157.54                                   | 43.28                                            | 20.72                                         | 24.56                |
| M1a        | -1205.238943            | 236.30                                  | 251.62                    | 170.83                                   | 43.44                                            | 17.65                                         | 22.93                |
| Di FF      |                        |                                         |                           |                                          |                                                  |                                               |                      |
| M1         | -1228.025646            | 215.76                                  | 230.05                    | 163.89                                   | 43.44                                            | 18.19                                         | 22.75                |
| M1a        | -1304.258939            | 231.39                                  | 247.17                    | 174.58                                   | 43.59                                            | 18.34                                         | 21.24                |
Table S3. Hydration Energies of FF and Fluorinated Derivatives at SMD(MP2/6-31G*).

| Molecule          | $\Delta E_{\text{water}}$ | $\Delta G_{\text{water}}$ | $\Delta W_{\text{water}}$ | $K_{\text{water}}$ | BR$^c$  |
|-------------------|---------------------------|---------------------------|---------------------------|---------------------|---------|
| $FF$              |                           |                           |                           |                     |         |
| M1 + H$_2$O → M1a | -12.90                    | -0.37                     | -2.54                     | 1.88                | 103.50  |
| Mono1 F-FF        |                           |                           |                           |                     |         |
| M1 + H$_2$O → M1a | -12.53                    | -1.48                     | -3.65                     | 474.27              | 26084.79|
| Mono2 F-FF        |                           |                           |                           |                     |         |
| M1 + H$_2$O → M1a | -13.77                    | -2.30                     | -4.47                     | 1869.28             | 102810.57|
| Di F-FF           |                           |                           |                           |                     |         |
| M1 + H$_2$O → M1a | -13.73                    | -2.03                     | -4.20                     | 1188.34             | 65358.65|

a) Hydration energies in kcal/mol.
b) Equilibrium constant $K_{\text{water}}$ computed with $\Delta W_{\text{water}} = -RT\cdot\ln(K_{\text{water}})$ at room temperature.
c) Bridging ratio BR = [bridged]/[unbridged] computed as product $K_{\text{water}} \cdot [H_2O]$. 

Figure S22. Minima of mono1 F-FF, unbridged structure (top) and bridged structure (bottom).
Figure S23. Minima of mono2 F-FF, unbridged structure (top) and bridged structure (bottom).
Figure S24a. Contact ion pair and neutral structures of FF, with relative energies $\Delta E$ and $\Delta G$ with respect to M3.
**Figure S24b.** Contact ion pair and neutral structures of mono1 F-FF, with relative energies $\Delta E$ and $\Delta G$ with respect to M3.
Figure S24c. Contact ion pair and neutral structures of mono2 F-FF, with relative energies $\Delta E$ and $\Delta G$ with respect to M3.
**Figure S24d.** Contact ion pair and neutral structures of di F-FF, with relative energies $\Delta E$ and $\Delta G$ with respect to M3.
Figure S25. M1 and M1a structures calculated at SMD(MP2/6-31G*) level.
Cartesian Coordinates of Stationary Structures at SMD(B3LYP/6-31G*)

Parent FF

Without water

M1

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X           | Y           | Z           |
| 1             | 8             | 0           | -0.606696   | 1.577118   | -0.914117   |
| 2             | 8             | 0           | 1.537035    | 3.740619   | -0.224126   |
| 3             | 8             | 0           | 3.192464    | 2.884678   | -1.491570   |
| 4             | 7             | 0           | -2.512485   | 2.546764   | 0.644666    |
| 5             | 7             | 0           | 0.862804    | 1.298367   | 0.822866    |
| 6             | 6             | 0           | -1.498352   | 1.662296   | 1.315187    |
| 7             | 6             | 0           | -2.147576   | 0.328853   | 1.751410    |
| 8             | 6             | 0           | -2.783361   | -0.484630  | 0.642131    |
| 9             | 6             | 0           | -2.034553   | -1.428067  | -0.076137   |
| 10            | 6             | 0           | -2.618575   | -2.169096  | -1.104666   |
| 11            | 6             | 0           | -3.963662   | -1.977199  | -1.432063   |
| 12            | 6             | 0           | -4.721521   | -1.045494  | -0.719370   |
| 13            | 6             | 0           | -4.135414   | -0.307978  | 0.312273    |
| 14            | 6             | 0           | -0.352156   | 1.514049   | 0.047646    |
| 15            | 6             | 0           | 2.106731    | 1.394249   | 0.047646    |
| 16            | 6             | 0           | 2.306561    | 0.233344   | -0.947372   |
| 17            | 6             | 0           | 2.449943    | -1.141610  | -0.326525   |
| 18            | 6             | 0           | 1.612418    | -2.194080  | -0.722068   |
| 19            | 6             | 0           | 1.759106    | -3.476783  | -0.184251   |
| 20            | 6             | 0           | 2.751520    | -3.729353  | 0.764043    |
| 21            | 6             | 0           | 3.597262    | -2.690481  | 1.165172    |
| 22            | 6             | 0           | 3.448282    | -1.412951  | 0.623306    |
| 23            | 6             | 0           | 2.274373    | 2.803085   | -0.627162   |
| 24            | 1             | 0           | -2.190569   | 3.521306   | 0.619642    |
| 25            | 1             | 0           | -3.420803   | 2.518512   | 1.122357    |
| 26            | 1             | 0           | -2.630513   | 2.237116   | -0.330734   |
| 27            | 1             | 0           | 0.945808    | 1.390177   | 1.828358    |
| 28            | 1             | 0           | -1.158521   | 2.195862   | 2.204292    |
| 29            | 1             | 0           | -1.361711   | -0.247867  | 2.249149    |
| 30            | 1             | 0           | -2.896542   | 0.575519   | 2.512572    |
| 31            | 1             | 0           | -0.990327   | -1.587989  | 0.178152    |
| 32            | 1             | 0           | -2.024090   | -2.899504  | -1.647098   |
| 33            | 1             | 0           | -4.419323   | -2.555051  | -2.231435   |
| 34            | 1             | 0           | 5.770699    | -0.896555  | -0.959753   |
| 35            | 1             | 0           | -4.735734   | 0.404587   | 0.874116    |
| 36            | 1             | 0           | 2.905473    | 1.340415   | 0.794744    |
| 37            | 1             | 0           | 3.215749    | 0.475501   | -1.505987   |
| 38            | 1             | 0           | 1.484339    | 0.227822   | -1.668684   |
| 39            | 1             | 0           | 0.840657    | -2.007945  | -1.465287   |
| 40            | 1             | 0           | 1.090208    | -4.276031  | -0.509420   |
| 41            | 1             | 0           | 2.868585    | -4.724543  | 1.184391    |
| 42            | 1             | 0           | 4.378284    | -2.876691  | 1.897911    |
| 43            | 1             | 0           | 4.121078    | -0.618784  | 0.938994    |

Rotational constants (GHz):
0.2958733
0.2070111
0.1401292

M1-CIP

S40
| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|------------------------|
|               |               |             | X          | Y            | Z            |
| 1             | 8             | 0           | -0.497053 | 0.015780    | -0.591677    |
| 2             | 8             | 0           | 0.077152  | 3.218331    | -0.204803    |
| 3             | 8             | 0           | 1.892800  | 3.444616    | -1.506422    |
| 4             | 7             | 0           | -2.005724 | 1.940112    | 1.137949     |
| 5             | 7             | 0           | 0.967485  | 0.911871    | 0.929667     |
| 6             | 6             | 0           | -1.355117 | 0.646662    | 1.581503     |
| 7             | 6             | 0           | -2.367019 | -0.497769   | 1.770591     |
| 8             | 6             | 0           | -3.293986 | -0.837517   | 0.618677     |
| 9             | 6             | 0           | -2.996309 | -1.882749   | -0.268657    |
| 10            | 6             | 0           | -3.868221 | -2.208840   | -1.307677    |
| 11            | 6             | 0           | -5.056561 | -1.492578   | -1.480550    |
| 12            | 6             | 0           | -5.370295 | -0.456456   | -0.599809    |
| 13            | 6             | 0           | -4.98917  | -0.138625   | 0.446034     |
| 14            | 6             | 0           | -0.244155 | 0.450637    | 0.536170     |
| 15            | 6             | 0           | 1.881167  | 1.573811    | -0.010875    |
| 16            | 6             | 0           | 2.488267  | 0.649037    | -1.089270    |
| 17            | 6             | 0           | 3.232400  | -0.543148   | -0.528154    |
| 18            | 6             | 0           | 2.623403  | -1.803741   | -0.449179    |
| 19            | 6             | 0           | 3.308997  | -2.900559   | 0.079326     |
| 20            | 6             | 0           | 4.619300  | -2.753395   | 0.540437     |
| 21            | 6             | 0           | 5.238260  | -1.502167   | 0.467471     |
| 22            | 6             | 0           | 4.549667  | -0.409605   | -0.063241    |
| 23            | 6             | 0           | 1.215021  | 2.847059    | -0.634491    |
| 24            | 1             | 0           | -2.156425 | 2.583913    | 0.767801     |
| 25            | 1             | 0           | -2.522448 | 2.381973    | 1.905773     |
| 26            | 1             | 0           | -2.663975 | 1.770399    | 0.367578     |
| 27            | 1             | 0           | 0.981818  | 1.328664    | 1.853296     |
| 28            | 1             | 0           | -0.914173 | 0.865033    | 2.555209     |
| 29            | 1             | 0           | -1.774271 | -1.376399   | 2.046848     |
| 30            | 1             | 0           | -2.968511 | -0.234831   | 2.648501     |
| 31            | 1             | 0           | -2.074459 | -2.443457   | -0.140896    |
| 32            | 1             | 0           | -3.621206 | -3.024510   | -1.981908    |
| 33            | 1             | 0           | -5.735013 | -1.746825   | -2.290222    |
| 34            | 1             | 0           | -6.297149 | 0.098628    | -0.716122    |
| 35            | 1             | 0           | -4.766110 | 0.651477    | 1.144775     |
| 36            | 1             | 0           | 2.707878  | 1.940810    | 0.606665     |
| 37            | 1             | 0           | 3.174201  | 1.275308    | -1.666234    |
| 38            | 1             | 0           | 1.700475  | 0.315009    | -1.767989    |
| 39            | 1             | 0           | 1.603275  | -1.924329   | -0.805465    |
| 40            | 1             | 0           | 2.819640  | -3.869957   | 0.128162     |
| 41            | 1             | 0           | 5.154965  | -3.605925   | 0.949344     |
| 42            | 1             | 0           | 6.259717  | -1.378362   | 0.818000     |
| 43            | 1             | 0           | 5.040827  | 0.559337    | -0.123955    |

Rotational constants (GHZ): 0.3821604 0.1492470 0.1217597

M1-N1
### Standard basis: 6-31G(d) (6D, 7F)

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|------------------------|
|               |               | X           | Y                      | Z                      |
| 1             | 8             | 0           | -0.880014              | 1.678235               | -0.332611               |
| 2             | 8             | 0           | 1.263872               | 3.791434               | 0.189655                |
| 3             | 8             | 0           | 1.659723               | 3.080697               | -1.912961               |
| 4             | 7             | 0           | -2.466240              | 1.532772               | 2.083440                |
| 5             | 7             | 0           | 0.918010               | 1.142044               | 0.940377                |
| 6             | 6             | 0           | -1.315284              | 0.662353               | 1.833520                |
| 7             | 6             | 0           | -1.771285              | -0.793634              | 1.538023                |
| 8             | 6             | 0           | -2.756999              | -0.959548              | 0.398726                |
| 9             | 6             | 0           | -2.320838              | -1.215700              | -0.910541               |
| 10            | 6             | 0           | -3.233818              | -1.374885              | -1.954823               |
| 11            | 6             | 0           | -4.606045              | -1.278993              | -1.708891               |
| 12            | 6             | 0           | -5.055651              | -1.028020              | -0.410522               |
| 13            | 6             | 0           | -4.138608              | -0.872729              | 0.631837                |
| 14            | 6             | 0           | -0.414362              | 1.195407               | 0.713259                |
| 15            | 6             | 0           | 1.907027               | 1.504176               | -0.070116               |
| 16            | 6             | 0           | 2.144717               | 0.404652               | -1.125823               |
| 17            | 6             | 0           | 2.712494               | -0.865585              | 0.527898                |
| 18            | 6             | 0           | 1.926266               | -2.017372              | -0.390808               |
| 19            | 6             | 0           | 2.453398               | -3.184100              | 0.170871                |
| 20            | 6             | 0           | 3.779485               | -3.215284              | 0.606186                |

Rotational constants (GHz):
- 0.4440538
- 0.1345749
- 0.1182037

Standard basis: 6-31G(d) (6D, 7F)
| Center | Atomic Number | Atomic Type | X     | Y     | Z     |
|--------|---------------|-------------|-------|-------|-------|
| 1      | 8             | 0           | 0.758863 | 1.539351 | 0.470682 |
| 2      | 8             | 0           | -2.227109 | 3.057982 | 1.769079 |
| 3      | 8             | 0           | -1.256307 | 3.781506 | -0.127812 |
| 4      | 7             | 0           | 2.435279  | 1.740563 | -1.901055 |
| 5      | 7             | 0           | -0.950180 | 1.114080 | -0.961213 |
| 6      | 6             | 0           | 1.341074  | 0.775144 | -1.763507 |
| 7      | 6             | 0           | 1.888090  | -0.664838 | -1.560151 |
| 8      | 6             | 0           | 2.868518  | -0.853146 | -0.419404 |
| 9      | 6             | 0           | 2.439070  | -1.264059 | 0.851858  |
| 10     | 6             | 0           | 3.349292  | -1.448238 | 1.694500  |
| 11     | 6             | 0           | 4.712341  | -1.222901 | 1.685140  |
| 12     | 6             | 0           | 5.155796  | -0.817252 | 0.424244  |
| 13     | 6             | 0           | 4.241799  | -0.637947 | -0.61791 |
| 14     | 6             | 0           | 0.364554  | 1.167277 | -0.647328 |
| 15     | 6             | 0           | -2.003122 | 1.466579 | -0.018058 |
| 16     | 6             | 0           | -2.245078 | 0.391289 | 1.067642  |
| 17     | 6             | 0           | -2.708363 | -0.927972 | 0.485607  |
| 18     | 6             | 0           | -1.839622 | -2.022725 | 0.386548  |
| 19     | 6             | 0           | -2.722243 | -3.235518 | -0.157514 |
| 20     | 6             | 0           | -3.585132 | -3.370628 | -0.613103 |
| 21     | 6             | 0           | -4.462634 | -2.286320 | -0.517972 |
| 22     | 6             | 0           | -4.026659 | -1.078004 | 0.027708  |
| 23     | 6             | 0           | -1.754557 | 2.880481 | 0.522265  |
| 24     | 1             | 0           | -2.092694 | 3.998600 | 2.003850  |
| 25     | 1             | 0           | 2.886613  | 1.829198 | -0.989765 |
| 26     | 1             | 0           | 2.027513  | 2.657656 | -0.087551 |
| 27     | 1             | 0           | -1.221419 | 0.822385 | -1.891174 |
| 28     | 1             | 0           | 0.790068  | 0.765115 | -2.709011 |
## M3

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|------------------------|
|               |               |             | X          | Y          | Z          |
| 1             | 8             | 0           | 0.130917   | -1.077315 | 0.568917   |
| 2             | 8             | 0           | -0.356222  | 3.112499  | -1.270452  |
| 3             | 8             | 0           | 0.910799   | 3.932633  | 0.409505   |
| 4             | 7             | 0           | -1.096638  | -2.684965 | -1.092975  |
| 5             | 7             | 0           | 0.420632   | 0.626794  | -0.934851  |
| 6             | 6             | 0           | -0.973342  | -1.263772 | -1.561792  |
| 7             | 6             | 0           | -2.367336  | -0.619304 | -1.737375  |
| 8             | 6             | 0           | -3.162294  | -0.415987 | -0.462720  |
| 9             | 6             | 0           | -3.038556  | 0.767626  | 0.275612   |
| 10            | 6             | 0           | -3.763577  | 0.950351  | 1.454517   |
| 11            | 6             | 0           | -4.622201  | -0.050339 | 1.912783   |
| 12            | 6             | 0           | -4.761076  | -1.236243 | 1.181969   |
| 13            | 6             | 0           | -4.036756  | -1.413505 | 0.001240   |
| 14            | 6             | 0           | -0.078585  | -0.551225 | -0.535283  |
| 15            | 6             | 0           | 1.052660   | 1.587821  | -0.033775  |
| 16            | 6             | 0           | 2.596577   | 1.590145  | 0.155798   |
| 17            | 6             | 0           | 3.248455   | 0.271144  | 0.195286   |
| 18            | 6             | 0           | 3.686711   | -0.608156 | -0.604547  |
| 19            | 6             | 0           | 4.269184   | -1.836235 | -0.477810  |
| 20            | 6             | 0           | 4.423711   | -2.204884 | 0.86005    |
| 21            | 6             | 0           | 3.994018   | -1.335629 | 1.867681   |
| 22            | 6             | 0           | 3.412709   | -0.111053 | 1.536289   |
| 23            | 6             | 0           | 0.480679   | 3.005750  | -0.325825  |
| 24            | 1             | 0           | -0.200652  | -3.178189 | -1.178866  |
| 25            | 1             | 0           | -1.803127  | -3.196387 | -1.633938  |
| 26            | 1             | 0           | -1.354568  | -2.704446 | -0.097751  |
| 27            | 1             | 0           | 0.024164   | 1.064577  | -1.764565  |
| 28            | 1             | 0           | -0.478816  | -1.301717 | -2.533872  |
| 29            | 1             | 0           | -2.201256  | 0.342968  | -2.231894  |
| 30            | 1             | 0           | -2.925588  | -1.245390 | -2.443181  |
| 31            | 1             | 0           | -2.378763  | 1.554323  | -0.082638  |
| 32            | 1             | 0           | -3.660035  | 1.877388  | 2.011910   |
| 33            | 1             | 0           | -5.190910  | 0.093999  | 2.828817   |
| 34            | 1             | 0           | -5.435888  | -2.012055 | 1.525306   |
| 35            | 1             | 0           | -4.159068  | -2.330141 | -0.571742  |
| 36            | 1             | 0           | 0.781008   | 1.318921  | 0.991586   |
| Center | Atomic Number | Atomic Number | Atomic Type | X     | Y     | Z     |
|--------|--------------|---------------|-------------|-------|-------|-------|
| 37     | 1            | 0             |             | 2.958543 | 2.378916 | 0.511183 |
| 38     | 1            | 0             |             | 2.864719 | 1.877905 | -1.179443 |
| 39     | 1            | 0             |             | 3.576216 | -0.325037 | -1.848727 |
| 40     | 1            | 0             |             | 4.064704 | -2.501540 | -1.269250 |
| 41     | 1            | 0             |             | 4.078656 | -3.157833 | 1.116669 |
| 42     | 1            | 0             |             | 4.115241 | -1.610718 | 2.912270 |
| 43     | 1            | 0             |             | 3.083839 | 0.560550  | 2.326427 |

Rotational constants (GHz): 0.3703007 0.1684556 0.1398062

With water

M1a

| Center | Atomic Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|--------|--------------|---------------|-------------|-------------------------|
| 1      | 8            | 0             |             | 0.828896 -1.026253 -0.871847 |
| 2      | 8            | 0             |             | -0.945201 -3.604979 -0.558527 |
| 3      | 8            | 0             |             | -2.281650 -2.814643 -2.170494 |
| 4      | 7            | 0             |             | 2.547461 -1.826133 1.115454 |
| 5      | 7            | 0             |             | -0.853550 -1.097751 0.671348 |
| 6      | 7            | 0             |             | 1.442119 -0.870414 1.457046 |
| 7      | 7            | 0             |             | 1.969669 0.561486 1.693284 |
| 8      | 6            | 0             |             | 2.718469 1.211208 0.547441 |
| 9      | 6            | 0             |             | 2.046325 2.014221 -0.385698 |
| 10     | 6            | 0             |             | 2.737066 2.619315 -1.436704 |
| 11     | 6            | 0             |             | 4.114981 2.429130 -1.572801 |
| 12     | 6            | 0             |             | 4.797068 1.637201 -0.646592 |
| 13     | 6            | 0             |             | 4.103688 1.037615 0.407780 |
| 14     | 6            | 0             |             | 0.431194 -0.997909 0.303388 |
| 15     | 6            | 0             |             | -1.941668 -1.401388 -0.258921 |
| 16     | 6            | 0             |             | -2.322187 -0.198857 -1.147703 |
| 17     | 6            | 0             |             | -2.838219 0.998703 -0.377905 |
| 18     | 6            | 0             |             | -2.137070 2.212021 -0.373149 |
| 19     | 6            | 0             |             | -2.614037 3.318656 0.336219 |
| 20     | 6            | 0             |             | -3.806625 3.228192 1.055986 |
| 21     | 6            | 0             |             | -4.520454 2.025542 1.055137 |
| 22     | 6            | 0             |             | -4.040892 0.925037 0.343689 |
| 23     | 6            | 0             |             | -1.676944 -2.709073 -1.077889 |
| 24     | 6            | 0             |             | 2.142101 -2.808435 1.097533 |
| 25     | 1            | 0             |             | 3.307755 -1.770386 1.801038 |
| 26     | 1            | 0             |             | 2.928666 -1.610483 0.187007 |
| 27     | 1            | 0             |             | -1.056071 -1.138142 1.665085 |
| 28     | 1            | 0             |             | 1.005605 -1.234359 2.383154 |
| 29     | 1            | 0             |             | 1.098513 1.165944 1.966459 |
| 30     | 1            | 0             |             | 2.615349 0.511050 2.577722 |
| 31     | 1            | 0             |             | 0.976079 2.171219 -0.279207 |
| 32     | 1            | 0             |             | 2.199976 3.241932 -2.147233 |
| 33     | 1            | 0             |             | 4.653497 2.901467 -2.389783 |
| 34     | 1            | 0             |             | 5.870163 1.492184 -0.737553 |
| 35     | 1            | 0             |             | 4.645232 0.438448 1.136666 |
| 36     | 1            | 0             |             | -2.800706 -1.638003 0.378525 |
| 37     | 1            | 0             |             | -3.091143 -0.555959 -1.838290 |
| 38     | 1            | 0             |             | -1.456835 0.088932 -1.752650 |
| 39     | 1            | 0             |             | -2.213251 2.293285 -0.940815 |
| 40     | 1            | 0             |             | -2.052933 4.249493 0.323945 |
| 41     | 1            | 0             |             | -4.180211 4.085955 1.608730 |
### M2b

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
| 1             | 8             | 0           | -0.626851, -0.037772, 1.275908 |
| 2             | 8             | 0           | -0.158193, 2.615552, -0.909254 |
| 3             | 8             | 0           | 1.114618, 3.599927, 0.676017 |
| 4             | 7             | 0           | -1.432509, -2.518120, 0.184391 |
| 5             | 7             | 0           | 0.927554, 0.133655, -0.373110 |
| 6             | 6             | 0           | -0.885042, -1.436046, -0.701699 |
| 7             | 6             | 0           | -1.989923, -0.839785, -1.611310 |
| 8             | 6             | 0           | -3.249796, -0.352953, -0.923506 |
| 9             | 6             | 0           | -3.335268, 0.939441, -0.382967 |
| 10            | 6             | 0           | -4.504059, 1.369347, 0.247901 |
| 11            | 6             | 0           | -5.60597, 0.516209, 0.347415 |
| 12            | 6             | 0           | -5.53591, -0.768736, -0.19418 |
| 13            | 6             | 0           | -4.366147, -1.196770, -0.826975 |
| 14            | 6             | 0           | -0.184197, -0.384849, 0.16907 |
| 15            | 6             | 0           | 1.581266, 1.316810, 0.179825 |
| 16            | 6             | 0           | 2.981482, 1.491336, -0.44648 |
| 17            | 6             | 0           | 3.921774, 0.328004, -0.215100 |
| 18            | 6             | 0           | 4.203454, -0.585255, -1.240533 |
| 19            | 6             | 0           | 5.059938, -1.668193, -1.023024 |
| 20            | 6             | 0           | 5.650354, -1.853390, 0.228622 |
| 21            | 6             | 0           | 5.379446, -0.947919, 1.259305 |
| 22            | 6             | 0           | 4.523309, 0.131820, 1.037659 |
| 23            | 6             | 0           | 0.752846, 2.623242, -0.035795 |
| 24            | 1             | 0           | -0.666139, -3.042869, 0.621075 |
| 25            | 1             | 0           | -1.984188, -3.183599, -0.369640 |
| 26            | 1             | 0           | -2.043302, -2.145437, 0.958975 |
| 27            | 1             | 0           | 1.182329, -0.151503, -1.313074 |
| 28            | 1             | 0           | -0.150684, -1.920915, -1.346360 |
| 29            | 1             | 0           | -1.515367, -0.023175, -2.165242 |
| 30            | 1             | 0           | -2.248159, -1.617222, -2.338430 |
| 31            | 1             | 0           | -2.485881, 1.612209, -0.461737 |
| 32            | 1             | 0           | -4.554891, 2.374367, 0.658291 |
| 33            | 1             | 0           | -6.515906, 0.853584, 0.837370 |
| 34            | 1             | 0           | -6.390251, -1.436872, -0.130907 |
| 35            | 1             | 0           | -4.319720, -2.195293, -1.256186 |
| 36            | 1             | 0           | 1.685321, 1.166271, 1.257611 |
| 37            | 1             | 0           | 3.398950, 2.407015, -0.016589 |
| 38            | 1             | 0           | 2.861693, 1.663582, -1.523763 |
| 39            | 1             | 0           | 3.752121, -0.441871, -2.219892 |
| 40            | 1             | 0           | 5.267069, -2.363166, -1.832633 |
| 41            | 1             | 0           | 6.319138, -2.692569, 0.399779 |
| 42            | 1             | 0           | 5.839303, -1.080713, 2.235155 |
| 43            | 1             | 0           | 4.321414, 0.834488, 1.843174 |
| 44            | 8             | 0           | -2.822837, -1.363701, 2.339105 |
| 45            | 1             | 0           | -2.148318, -0.678968, 2.153140 |
| 46            | 1             | 0           | -2.459242, -1.852017, 3.094749 |
Rotational constants (GHZ): 0.4411152 0.1207093 0.1075689

M3b

| Center Number | Atomic Number | Atomic Type | X            | Y            | Z            |
|---------------|---------------|-------------|--------------|--------------|--------------|
| 1             | 8             | 0           | -0.211689    | -0.984331    | -0.388014    |
| 2             | 8             | 0           | 0.061019     | 3.405326     | 1.010801     |
| 3             | 8             | 0           | -1.170823    | 3.965736     | -0.797541    |
| 4             | 7             | 0           | 1.136925     | -2.330273    | 1.531171     |
| 5             | 7             | 0           | -0.550552    | 0.859877     | 0.911099     |
| 6             | 6             | 0           | 0.924886     | -0.861811    | 1.757483     |
| 7             | 6             | 0           | 2.271302     | -0.108036    | 1.869997     |
| 8             | 6             | 0           | 3.096833     | -0.015311    | 0.603006     |
| 9             | 6             | 0           | 2.905901     | 1.045250     | 0.296495     |
| 10            | 6             | 0           | 3.664706     | 1.131499     | 1.465278     |
| 11            | 6             | 0           | 4.628865     | 0.160961     | 1.750410     |
| 12            | 6             | 0           | 4.833615     | -0.893117    | 0.857169     |
| 13            | 6             | 0           | 4.074163     | -0.977649    | 0.312026     |
| 14            | 6             | 0           | 0.000760     | -0.332119    | 0.650872     |
| 15            | 6             | 0           | -1.231250    | 1.684184     | -0.085055    |
| 16            | 6             | 0           | -2.773350    | 1.628396     | 0.048637     |
| 17            | 6             | 0           | 3.369458     | 0.257278     | 0.179999     |
| 18            | 6             | 0           | 3.768572     | 0.547891     | 0.895685     |
| 19            | 6             | 0           | -4.303392    | -1.821488    | 0.680682     |
| 20            | 6             | 0           | -4.448323    | -2.310695    | -0.619028    |
| 21            | 6             | 0           | -4.056340    | -1.516644    | -1.701426    |
| 22            | 6             | 0           | -3.522296    | -0.246433    | -1.481578    |
| 23            | 6             | 0           | -0.730222    | 3.151415     | 0.055315     |
| 24            | 1             | 0           | 0.251775     | -2.837431    | 1.640747     |
| 25            | 1             | 0           | 1.796266     | -2.701867    | 2.223559     |
| 26            | 1             | 0           | 1.494903     | -2.552790    | 0.567881     |
| 27            | 1             | 0           | 0.189559     | 1.406700     | 1.690533     |
| 28            | 1             | 0           | 0.413474     | -0.778668    | 2.718770     |
| 29            | 1             | 0           | 2.031644     | 0.897080     | 2.231827     |
| 30            | 1             | 0           | 2.847197     | -0.597179    | 2.663886     |
| 31            | 1             | 0           | 2.170260     | 1.813388     | -0.069855    |
| 32            | 1             | 0           | 3.507905     | 1.961237     | -2.149231    |
| 33            | 1             | 0           | 5.221771     | 0.230275     | -2.658296    |
| 34            | 1             | 0           | 5.588288     | -1.646464    | -1.065634    |
| 35            | 1             | 0           | 4.245644     | -1.793934    | 1.010057     |
| 36            | 1             | 0           | -0.948454    | 1.320595     | -1.077249    |
| 37            | 1             | 0           | -3.170363    | 2.337643     | -0.683097    |
| 38            | 1             | 0           | -3.049355    | 1.994806     | 1.04628      |
| 39            | 1             | 0           | -3.663292    | -0.170439    | 1.910453     |
| 40            | 1             | 0           | -4.609662    | -2.428016    | 1.529139     |
| 41            | 1             | 0           | -4.866938    | -3.299043    | -0.788873    |
| 42            | 1             | 0           | -4.170632    | -1.885916    | -2.717341    |
| 43            | 1             | 0           | -3.223445    | 0.368622     | -2.329030    |
| 44            | 8             | 0           | 1.681351     | -2.887062    | 1.187152     |
| 45            | 1             | 0           | 0.988584     | -2.193338    | -1.237397    |
| 46            | 1             | 0           | 1.178417     | -3.714599    | -1.279702    |

Rotational constants (GHZ): 0.3255179 0.1610784 0.1305382
**Mono1 F-FF**

Without water

**M1**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X           | Y           | Z               |
| 1             | 8             | 0           | 0.201162    | 1.416468    | 1.092665        |
| 2             | 8             | 0           | -1.879155   | 3.629357    | 0.270508        |
| 3             | 8             | 0           | -3.880653   | 2.831194    | 0.937911        |
| 4             | 7             | 0           | 2.174208    | 2.631949    | -0.128311       |
| 5             | 7             | 0           | -1.092781   | 1.242795    | -0.797836       |
| 6             | 6             | 0           | 1.268944    | 1.828128    | -1.019211       |
| 7             | 6             | 0           | 2.006942    | 0.607407    | -1.610955       |
| 8             | 6             | 0           | 2.581686    | -0.376609   | -0.614695       |
| 9             | 6             | 0           | 1.897904    | -1.541780   | 0.241140        |
| 10            | 6             | 0           | 2.451437    | -2.450792   | 0.662424        |
| 11            | 6             | 0           | 3.714523    | -2.213270   | 1.210200        |
| 12            | 6             | 0           | 4.424985    | -1.065500   | 0.853126        |
| 13            | 6             | 0           | 3.841435    | -0.184757   | -0.045436       |
| 14            | 6             | 0           | 2.051307    | 1.479809    | -0.137473       |
| 15            | 6             | 0           | -2.423738   | 1.298447    | -0.176852       |
| 16            | 6             | 0           | -2.692087   | 0.194410    | 0.869685        |
| 17            | 6             | 0           | -2.618877   | -1.220448   | 0.338560        |
| 18            | 6             | 0           | -1.588777   | -2.084718   | 0.732569        |
| 19            | 6             | 0           | -1.528887   | -3.398163   | 0.255802        |
| 20            | 6             | 0           | -2.502110   | -3.867787   | -0.628349       |
| 21            | 6             | 0           | -3.535932   | -3.015623   | -1.029404       |
| 22            | 6             | 0           | -3.592674   | -1.706791   | -0.548374       |
| 23            | 6             | 0           | -2.741880   | 2.721763    | 0.401858        |
| 24            | 1             | 0           | 1.867982    | 3.610412    | -0.081214       |
| 25            | 1             | 0           | 3.152473    | 2.609744    | -0.436073       |
| 26            | 1             | 0           | 2.105355    | 2.243106    | 0.825967        |
| 27            | 1             | 0           | -1.076168   | 1.455063    | -1.789232       |
| 28            | 1             | 0           | 0.969309    | 2.481732    | -1.839349       |
| 29            | 1             | 0           | 1.288013    | 0.093891    | -2.255520       |
| 30            | 1             | 0           | 2.798590    | 0.993864    | -2.261598       |
| 31            | 1             | 0           | 0.920451    | -1.733930   | -0.673334       |
| 32            | 1             | 0           | 1.899212    | -3.346196   | 0.932028        |
| 33            | 1             | 0           | 4.151482    | -2.917529   | 1.911730        |
| 34            | 1             | 0           | 5.409996    | -0.849488   | 1.253632        |
| 35            | 1             | 0           | -3.124816   | 1.147065    | -1.003659       |
| 36            | 1             | 0           | -3.699978   | 0.392324    | 1.246386        |
| 37            | 1             | 0           | -2.003406   | 0.312640    | 1.709945        |
| 38            | 1             | 0           | -0.723699   | -4.053090   | 0.579390        |
| 39            | 1             | 0           | -2.459528   | -4.888501   | -0.998680       |
| 40            | 1             | 0           | -4.302276   | -3.373493   | -1.712193       |
| 41            | 1             | 0           | -4.406440   | -1.054713   | -0.858761       |
| 42            | 9             | 0           | 4.541689    | 0.937780    | -0.392198       |
| 43            | 1             | 0           | -0.827793   | -1.724636   | 1.420655        |

Rotational constants (GHz): 0.2948492 0.1843368 0.1249135

**M1-CIP**
| Center Number | Atomic Number | Atomic Type | X        | Y        | Z        |
|---------------|---------------|-------------|----------|----------|----------|
| 1             | 8             | 0           | -0.400181| 0.122307 | -0.594821|
| 2             | 8             | 0           | 0.277343 | 3.293962 | -0.292122|
| 3             | 8             | 0           | 2.089267 | 3.423248 | -1.612115|
| 4             | 7             | 0           | -1.829919| 2.128388 | 1.122966 |
| 5             | 7             | 0           | 1.101601 | 0.994480 | 0.903864 |
| 6             | 6             | 0           | -1.224553| 0.811892 | 1.571983 |
| 7             | 6             | 0           | -2.264322| -0.298259| 1.789253 |
| 8             | 6             | 0           | -2.967999| -0.911015| 0.594405 |
| 9             | 6             | 0           | -2.654100| -2.200303| 0.140859 |
| 10            | 6             | 0           | -3.345435| -2.789038| -0.919421|
| 11            | 6             | 0           | -4.380839| -2.096744| -1.552136|
| 12            | 6             | 0           | -4.723097| -0.813467| -1.121413|
| 13            | 6             | 0           | -4.012557| -0.264960| -0.064718|
| 14            | 6             | 0           | -0.125172| 0.563893 | 0.525217 |
| 15            | 6             | 0           | 2.031789 | 1.602555 | -0.056180|
| 16            | 6             | 0           | 2.610903 | 0.627811 | -1.105923|
| 17            | 6             | 0           | 3.314782 | -0.571159| -0.508528|
| 18            | 6             | 0           | 2.664293 | -1.808135| -0.393979|
| 19            | 6             | 0           | 3.313145 | -2.911335| 0.166624 |
| 20            | 6             | 0           | 4.627453 | -2.794272| 0.625013 |
| 21            | 6             | 0           | 5.287391 | 1.566732 | 0.571110 |
| 22            | 6             | 0           | 4.635460 | -0.467719| -0.045660|
| 23            | 6             | 0           | 1.400141 | 2.874925 | -0.717106|
| 24            | 1             | 0           | -1.066144| 2.725713 | 0.707636 |
| 25            | 1             | 0           | -2.275950| 2.611520 | 1.901008 |
| 26            | 1             | 0           | -2.546304| 1.985255 | 0.402723 |
| 27            | 1             | 0           | 1.138149 | 1.424600 | 1.820838 |
| 28            | 1             | 0           | -0.775609| 1.026772 | 2.542682 |
| 29            | 1             | 0           | -1.731457| -1.095251| 2.371979 |
| 30            | 1             | 0           | -3.006582| 0.097308 | 2.493390 |
| 31            | 1             | 0           | -1.853913| -2.744847| 0.634859 |
| 32            | 1             | 0           | -3.077973| -3.788906| -1.247820|
| 33            | 1             | 0           | -4.922976| -2.548987| -2.377101|
| 34            | 1             | 0           | -5.522308| -0.243688| -1.584029|
| 35            | 1             | 0           | 2.869185 | 1.964503 | 0.549853 |
| 36            | 1             | 0           | 3.318040 | 1.213747 | -1.69270 |
| 37            | 1             | 0           | 1.813979 | 0.293953 | -1.776770|
| 38            | 1             | 0           | 2.792081 | -3.862288| 0.242597 |
| 39            | 1             | 0           | 5.134530 | -3.651922| 1.058893 |
| 40            | 1             | 0           | 6.312195 | -1.466652| 0.865425 |
| 41            | 1             | 0           | 5.158308 | 0.482374 | -0.133533|
| 42            | 9             | 0           | -4.350556| 0.996580 | 0.350288 |
| 43            | 1             | 0           | 1.640837 | -1.905249| -0.748007|

Rotational constants (GHZ): 0.3417853 0.1461852 0.1159651

Standard basis: 6-31G(d) (6D, 7F)

**M1-N1**

| Center Number | Atomic Number | Atomic Type | X        | Y        | Z        |
|---------------|---------------|-------------|----------|----------|----------|
| 1             | 8             | 0           | 0.092742 | -0.408839| 0.733936 |
| 2             | 8             | 0           | -0.010275| 3.053670 | 0.023249 |
| 3             | 8             | 0           | -1.705344| 3.430853 | 1.391455 |
| 4             | 7             | 0           | 1.668402 | 1.313039 | -1.420199|
| 5             | 7             | 0           | -1.119034| 0.670811 | -0.885917|

S49
| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               | 6             | 0           | X                       |
| 1             | 18            | 0           | 0.470958                |
| 2             | 18            | 0           | -1.781366               |
| 3             | 18            | 0           | -2.339252               |
| 4             | 17            | 0           | 2.269193                |
| 5             | 7             | 0           | -1.168040               |
| 6             | 6             | 0           | 1.159281                |
| 7             | 6             | 0           | 1.674468                |
| 8             | 6             | 0           | 2.596892                |
| 9             | 6             | 0           | 2.118699                |
| 10            | 6             | 0           | 2.985532                |
| 11            | 6             | 0           | 4.367889                |
| 12            | 6             | 0           | 4.877423                |
| 13            | 6             | 0           | 3.985807                |
| Center Number | Atomic Number | Atomic Type | X (Angstroms) | Y (Angstroms) | Z (Angstroms) |
|---------------|---------------|-------------|---------------|---------------|---------------|
| 1             | 8             | 0           | 0.388556      | 1.720940      | 0.524588      |
| 2             | 8             | 0           | -2.724595     | 2.981608      | 1.667580      |
| 3             | 8             | 0           | -1.782204     | 3.751133      | -0.225987     |
| 4             | 7             | 0           | 2.218939      | 1.844812      | -1.719370     |
| 5             | 7             | 0           | -1.206417     | 1.092111      | -0.963078     |
| 6             | 6             | 0           | 1.140758      | 0.858338      | -1.623300     |
| 7             | 6             | 0           | 1.702374      | -0.563592     | -1.343292     |
| 8             | 6             | 0           | 2.641433      | -0.684877     | -0.161952     |
| 9             | 6             | 0           | 2.185875      | -0.901896     | 1.147917      |
| 10            | 6             | 0           | 3.069966      | -1.024805     | 2.220904      |
| 11            | 6             | 0           | 4.447729      | -0.935447     | 2.005677      |
| 12            | 6             | 0           | 4.935420      | -0.728942     | 0.714850      |
| 13            | 6             | 0           | 4.026781      | -0.609117     | -0.329786     |
| 14            | 6             | 0           | 0.081883      | 1.254205      | -0.585246     |
| 15            | 6             | 0           | -2.331950     | 1.384323      | -0.084582     |
| 16            | 6             | 0           | -2.550782     | 0.317373      | 1.013264      |
| 17            | 6             | 0           | -2.841676     | -1.055433     | 0.442106      |
| 18            | 6             | 0           | -1.907525     | -2.094643     | 0.544656      |
| 19            | 6             | 0           | -2.178966     | -3.359250     | 0.013748      |
| 20            | 6             | 0           | -3.392999     | -3.602661     | -0.631140     |
| 21            | 6             | 0           | -4.334958     | -2.574793     | -0.737239     |

Rotational constants (GHZ): 0.3034694 0.1561783

Standard basis: 6-31G(d) (6D, 7F)

**M1-N3**

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S51
| Center | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|--------|---------------|-------------|-------------------------|
| 1      | 8             | 0           | X: 0.392551 Y: -1.030256 Z: 0.703466 |
| 2      | 8             | 0           | X: 0.018571 Y: 3.155540 Z: -1.348094 |
| 3      | 8             | 0           | X: 1.280729 Y: 3.973759 Z: 0.337337 |
| 4      | 7             | 0           | X: -1.065376 Y: -2.614910 Z: -0.732537 |
| 5      | 7             | 0           | X: 0.580784 Y: 0.650311 Z: -0.838574 |
| 6      | 6             | 0           | X: -0.837752 Y: -1.262842 Z: -1.357637 |
| 7      | 6             | 0           | X: -2.164123 Y: -0.526268 Z: -1.644173 |
| 8      | 6             | 0           | X: -2.979131 Y: -0.128609 Z: -0.430630 |
| 9      | 6             | 0           | X: -2.901434 Y: 1.155123 Z: 0.130011 |
| 10     | 6             | 0           | X: -3.678890 Y: 1.510219 Z: 1.234123 |
| 11     | 6             | 0           | X: -4.561227 Y: 0.586302 Z: 1.799114 |
| 12     | 6             | 0           | X: -4.664933 Y: -0.698512 Z: 1.261896 |
| 13     | 6             | 0           | X: -3.874675 Y: -1.014713 Z: 0.168078 |
| 14     | 6             | 0           | X: 0.110392 Y: -0.516757 Z: -0.393828 |
| 15     | 6             | 0           | X: 1.321242 Y: 1.611975 Z: 0.024486 |
| 16     | 6             | 0           | X: 2.853277 Y: 1.525590 Z: -0.243087 |
| 17     | 6             | 0           | X: 3.466420 Y: 0.193598 Z: 0.127214 |
| 18     | 6             | 0           | X: 3.793468 Y: -0.749651 Z: -0.856756 |
| 19     | 6             | 0           | X: 4.341957 Y: -1.988161 Z: -0.511340 |
| 20     | 6             | 0           | X: 4.573489 Y: -2.302733 Z: 0.829124 |
| 21     | 6             | 0           | X: 4.255311 Y: -1.369150 Z: 1.820544 |
| 22     | 6             | 0           | X: 3.707631 Y: -0.134306 Z: 1.470797 |
| 23     | 6             | 0           | X: 0.820892 Y: 3.043389 Z: -0.374119 |
| 24     | 6             | 0           | X: -0.635002 Y: -3.364645 Z: -1.28234 |
| 25     | 6             | 0           | X: -2.062220 Y: -2.834598 Z: -0.616161 |
| 26     | 6             | 0           | X: -0.612522 Y: -2.586390 Z: 0.202207 |
| 27     | 6             | 0           | X: 0.157126 Y: 1.079871 Z: -1.659366 |
| 28     | 6             | 0           | X: -0.325081 Y: -1.430885 Z: -2.305852 |
| 29     | 6             | 0           | X: -1.911535 Y: 0.370967 Z: -2.215797 |
| Center | Atomic Number | Atomic Type | Coordinates (Angstroms) | X     | Y     | Z      |
|--------|---------------|-------------|-------------------------|-------|-------|--------|
| 30     | 1             | 0           | -2.754473               | -1.163577 | -2.310994 |
| 31     | 1             | 0           | -2.222426               | 1.879060  | -0.312494 |
| 32     | 1             | 0           | -3.599861               | 2.510885  | 1.647986  |
| 33     | 1             | 0           | -5.169373               | 0.859323  | 2.656210  |
| 34     | 1             | 0           | -5.339243               | -1.442910 | 1.672163  |
| 35     | 1             | 0           | 1.099178                | 1.415772  | 1.022824  |
| 36     | 1             | 0           | 3.295479                | 2.324341  | 0.361052  |
| 37     | 1             | 0           | 3.065195                | 1.754047  | -1.294600 |
| 38     | 1             | 0           | 4.590809                | -2.703849 | -1.290691 |
| 39     | 1             | 0           | 5.002347                | -3.263776 | 1.100069  |
| 40     | 1             | 0           | 4.437836                | -1.602112 | 2.866436  |
| 41     | 1             | 0           | 3.466267                | 0.587798  | 2.247829  |
| 42     | 9             | 0           | -3.971063               | -2.280834 | -0.351456 |

Rotational constants (GHz): 0.3495518 0.1522307 0.1236029

With water

M1a

| Center | Atomic Number | Atomic Type | Coordinates (Angstroms) | X     | Y     | Z      |
|--------|---------------|-------------|-------------------------|-------|-------|--------|
| 1      | 8             | 0           | 0.503776                | 1.028860 | 0.976307 |
| 2      | 8             | 0           | -1.322234               | 3.572689 | 0.604099 |
| 3      | 8             | 0           | -2.677172               | 2.726652 | 2.175302 |
| 4      | 7             | 0           | 2.267819                | 1.921981 | -0.928914 |
| 5      | 7             | 0           | -1.114123               | 1.078719 | -0.637354 |
| 6      | 6             | 0           | 1.218836                | 0.923871 | -1.318414 |
| 7      | 6             | 0           | 1.801515                | -0.489984 | -1.532022 |
| 8      | 6             | 0           | 2.564199                | -1.095869 | -0.374114 |
| 9      | 6             | 0           | 1.962829                | -1.962890 | 0.549099 |
| 10     | 6             | 0           | 2.694772                | -2.534771 | 1.590936 |
| 11     | 6             | 0           | 4.055976                | -2.250627 | 1.729121 |
| 12     | 6             | 0           | 4.685605                | -1.394921 | 0.823435 |
| 13     | 6             | 0           | 3.926048                | -0.844055 | -0.198968 |
| 14     | 6             | 0           | 0.155469                | 1.007835  | -0.214734 |
| 15     | 6             | 0           | -2.244338               | 1.343846  | 0.256375 |
| 16     | 6             | 0           | -2.621739               | 0.125487  | 1.125178 |
| 17     | 6             | 0           | -3.021077               | -1.098411 | 0.328753 |
| 18     | 6             | 0           | -2.323152               | -2.256606 | 0.342187 |
| 19     | 6             | 0           | -2.597657               | -3.387335 | -0.394635 |
| 20     | 6             | 0           | -3.764266               | -3.376487 | -1.161275 |
| 21     | 6             | 0           | -4.564216               | -2.229229 |
| 22     | 6             | 0           | -4.195779               | -1.104580 | -0.440682 |
| 23     | 6             | 0           | -2.042066               | 2.650694  | 1.094137 |
| 24     | 1             | 0           | 1.826841                | 2.888146  | -0.970384 |
| 25     | 1             | 0           | 3.086630                | 1.874092  | -1.542882 |
| 26     | 1             | 0           | 2.570814                | 1.747859  | 0.037001 |
| 27     | 1             | 0           | -1.277597               | 1.128074  | -1.635056 |
| 28     | 1             | 0           | 0.809619                | 1.271203  | -2.268103 |
| 29     | 1             | 0           | 0.955917                | -1.135378 | -1.788426 |
| 30     | 1             | 0           | 2.445781                | -0.439506 | -2.416028 |
| 31     | 1             | 0           | 0.907347                | -2.193573 | 0.434741 |
| 32     | 1             | 0           | 2.204165                | -3.204537 | 2.290752 |
| 33     | 1             | 0           | 4.630913                | -2.693890 | 2.536674 |
| 34     | 1             | 0           | 5.741306                | -1.154922 | 0.896496 |

S53
Rotational constants (GHZ):  
0.2520610  
0.1568207  
0.1143770  

Center  Atomic  Atomic  Coordinates (Angstroms)  
Number  Number  Type            X         Y         Z  
-------  --------  -----  ---------  ----------  ----------  ----------  
1         8        0     -0.370869  -0.030320  1.260587  
2         8        0     0.084757   2.63975    -1.055654  
3         8        0     1.438349   3.651256   0.442977  
4         7        0     -1.378772  -2.403213   0.083688  
5         7        0     1.099507   0.155065  -0.465748  
6         6        0     -0.805334  -1.305303  -0.766068  
7         6        0     -1.913220  -0.573752  -1.565526  
8         6        0     -3.074756  -0.035799  -0.758527  
9         6        0     -3.099400  1.268049  -0.241897  
10        6        0     -4.191364   1.732461   0.493811  
11        6        0     -5.288380   0.898756   0.727231  
12        6        0     -5.295938  -0.403399  0.221218  
13        6        0     -4.195533  -0.831736  -0.505275  
14        6        0     -0.002146  -0.342004   0.113841  
15        6        0     1.796137   1.325690   0.061403  
16        6        0     3.213530   1.420185  -0.542765  
17        6        0     4.112678   0.249444  -0.209158  
18        6        0     4.379592  -0.750083  -1.154768  
19        6        0     5.196326  -1.839122  -0.837594  
20        6        0     5.761337  -1.943838   0.435045  
21        6        0     5.505502  -0.951511   1.386452  
22        6        0     4.689053   0.139397   1.065281  
23        6        0     1.020019   2.654933  -0.207345  
24        1        0     -0.631734  -3.020716   0.421184  
25        1        0     -2.030156  -2.975500  -0.465378  
26        1        0     -1.894341  -2.043056   0.930963  
27        1        0     1.269345  -0.082802  -1.437440  
28        1        0     -0.140653  -1.791715  -1.481532  
29        1        0     -1.418989   0.247787  -2.091862  
30        1        0     -2.277815  -1.273537  -2.323402  
31        1        0     -2.248525   1.918884  -0.423115  
32        1        0     -4.186567   2.746319   0.882478  
33        1        0     -6.139833   1.256603   1.298328  
34        1        0     -6.130954  -1.078213   0.376347  
35        1        0     1.874025   1.203242   1.144330  
36        1        0     3.648873   2.349950  -0.163904  
37        1        0     3.123007   1.523995  -1.631601  
38        1        0     5.392058  -2.602594  -1.586043  
39        1        0     6.398697  -2.788165   0.683444  
40        1        0     5.945815  -1.021051   2.377745  

M2b
| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|------------------------|
| 1             | 8             | 0           | 0.367725               |
| 2             | 8             | 0           | -0.933251              |
| 3             | 8             | 0           | 3.422316               |
| 4             | 7             | 0           | -1.116626              |
| 5             | 7             | 0           | -0.61935                |
| 6             | 6             | 0           | -0.61935                |
| 7             | 6             | 0           | 1.512423               |
| 8             | 6             | 0           | -0.139800               |
| 9             | 6             | 0           | 1.42531                |
| 10            | 6             | 0           | 1.100127               |
| 11            | 6             | 0           | -0.61935                |
| 12            | 6             | 0           | 1.100127               |
| 13            | 6             | 0           | -0.61935                |
| 14            | 6             | 0           | 0.021551               |
| 15            | 6             | 0           | -0.61935                |
| 16            | 6             | 0           | 1.512423               |
| 17            | 6             | 0           | -0.139800               |
| 18            | 6             | 0           | 1.42531                |
| 19            | 6             | 0           | -0.61935                |
| 20            | 6             | 0           | 1.512423               |
| 21            | 6             | 0           | -0.139800               |
| 22            | 6             | 0           | 1.42531                |
| 23            | 6             | 0           | 1.100127               |
| 24            | 1             | 0           | -0.17851               |
| 25            | 1             | 0           | -0.17851               |
| 26            | 1             | 0           | 1.512423               |
| 27            | 1             | 0           | -0.139800               |
| 28            | 1             | 0           | 1.42531                |
| 29            | 1             | 0           | -0.61935                |
| 30            | 1             | 0           | 1.512423               |
| 31            | 1             | 0           | -0.139800               |
| 32            | 1             | 0           | 1.512423               |
| 33            | 1             | 0           | -0.139800               |
| 34            | 1             | 0           | 1.512423               |
| 35            | 1             | 0           | -0.139800               |
| 36            | 1             | 0           | 1.512423               |
| 37            | 1             | 0           | -0.139800               |
| 38            | 1             | 0           | 1.512423               |
| 39            | 1             | 0           | -0.139800               |
| 40            | 1             | 0           | 1.512423               |
| 41            | 1             | 0           | -0.139800               |
| 42            | 8             | 0           | -0.933251              |
| 43            | 1             | 0           | -0.933251              |
| 44            | 9             | 0           | -0.933251              |
| 45            | 1             | 0           | -0.933251              |
| 46            | 1             | 0           | -0.933251              |

**Rotational constants (GHZ):**

0.4009587
0.1127083

**M3b**
Rotational constants (GHZ):    0.3085523    0.1467616
0.1195913

**Mono2 F-FF**

*Without water*

**M1**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|------------------------|
|               |               | X           | Y                      | Z                      |
| 1             | 8             | 0           | 0.891186               | 1.567823               | 0.544114               |
| 2             | 8             | 0           | -1.070445              | 3.884760               | -0.120006              |
| 3             | 8             | 0           | -2.173429              | 3.263345               | 1.744660               |
| 4             | 7             | 0           | 2.582319               | 1.816046               | -1.593816              |
| 5             | 7             | 0           | -0.834763              | 1.237516               | -0.920540              |
| 6             | 6             | 0           | 1.444689               | 0.835184               | -1.676054              |
| 7             | 6             | 0           | 1.971400               | -0.616089              | -1.544054              |
| 8             | 6             | 0           | 2.937507               | -0.880050              | -0.403232              |
| 9             | 6             | 0           | 2.490077               | -1.269979              | 0.868583               |
| 10            | 6             | 0           | 3.399176               | -1.512263              | 1.899750               |
| 11            | 6             | 0           | 4.771507               | -1.366764              | 1.679604               |
| 12            | 6             | 0           | 5.229933               | -0.984464              | 0.47528                |
| 13            | 6             | 0           | 4.318864               | -0.748189              | -0.614575              |
| 14            | 6             | 0           | 0.458590               | 1.248212               | -0.574977              |
| 15            | 6             | 0           | -1.917176              | 1.626428               | -0.011277              |
| 16            | 6             | 0           | -2.226029              | 0.536322               | 1.037473               |
| 17            | 6             | 0           | -2.836812              | -0.714766              | 0.448507               |
| 18            | 6             | 0           | -2.068712              | -1.805020              | 0.039971               |
| 19            | 6             | 0           | -2.599645              | -2.961674              | -0.515914              |
| 20            | 6             | 0           | -3.982725              | -3.046498              | -0.683199              |
| 21            | 6             | 0           | -4.795534              | -1.979827              | -0.290200              |
| 22            | 6             | 0           | -4.223941              | -0.835493              | 0.268651               |
| 23            | 6             | 0           | -1.675470              | 3.050403               | 0.605128               |
| 24            | 1             | 0           | 2.288796               | 2.750934               | -1.902139              |
| 25            | 1             | 0           | 3.379698               | 1.523952               | -2.170835              |
| 26            | 1             | 0           | 2.895237               | 1.894360               | -0.61615               |
| 27            | 1             | 0           | -1.070758              | 0.994455               | -1.874699              |
| 28            | 1             | 0           | 1.000652               | 0.959750               | -2.664342              |
| 29            | 1             | 0           | 1.089958               | -1.258161              | -1.460139              |
| 30            | 1             | 0           | 2.460442               | -0.857282              | -2.493961              |
| 31            | 1             | 0           | 1.427521               | -1.394198              | 1.049778               |
| 32            | 1             | 0           | 3.034116               | -1.818729              | 2.876337               |
| 33            | 1             | 0           | 5.477358               | -1.556902              | 2.483442               |
| 34            | 1             | 0           | 6.295146               | -0.877794              | 0.231243               |
| 35            | 1             | 0           | -2.799251              | 1.738976               | -0.651459              |
| 36            | 1             | 0           | -2.932032              | 0.973178               | 1.746384               |
| 37            | 1             | 0           | -1.312502              | 0.300333               | 1.590855               |
| 38            | 1             | 0           | -1.935582              | -3.770056              | -0.804925              |
| 39            | 1             | 0           | -4.418551              | -3.942207              | -1.115829              |
| 40            | 1             | 0           | -5.872919              | -2.040924              | -0.413177              |
| 41            | 1             | 0           | -4.860255              | -0.010791              | 0.580732               |
| 42            | 9             | 0           | -0.713009              | -1.743860              | 0.194487               |
| 43            | 1             | 0           | 4.684423               | -0.469355              | -1.600963              |

Rotational constants (GHZ):    0.3195690    0.1647050
0.1277994

S56
### M1-CIP

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X           | Y           | Z           |
| 1             | 8             | 0           | -0.601550   | -0.170235   | -0.674512   |
| 2             | 8             | 0           | -0.449536   | 3.017829    | 0.153133    |
| 3             | 8             | 0           | 1.025636    | 3.347843    | -1.459498   |
| 4             | 7             | 0           | -1.912614   | 1.254691    | 1.790062    |
| 5             | 7             | 0           | -0.808795   | 0.643315    | 0.927478    |
| 6             | 6             | 0           | -1.366291   | -0.118512   | 1.647091    |
| 7             | 6             | 0           | -2.397933   | -1.257232   | 1.462711    |
| 8             | 6             | 0           | -3.513727   | -1.038115   | 0.459089    |
| 9             | 6             | 0           | -3.464160   | -1.598699   | -0.826581   |
| 10            | 6             | 0           | -4.506600   | -1.407789   | -1.734809   |
| 11            | 6             | 0           | -5.623115   | -0.647377   | -1.375569   |
| 12            | 6             | 0           | -5.692118   | -0.090498   | -0.097282   |
| 13            | 6             | 0           | -4.649938   | -0.291526   | 0.812196    |
| 14            | 6             | 0           | -0.350837   | 0.049721    | 0.512809    |
| 15            | 6             | 0           | 1.558898    | 1.551659    | 0.065621    |
| 16            | 6             | 0           | 2.371373    | 0.864599    | -1.054813   |
| 17            | 6             | 0           | 3.421698    | -0.080697   | -0.519888   |
| 18            | 6             | 0           | 3.188487    | -1.451815   | -0.402811   |
| 19            | 6             | 0           | 4.127855    | -2.349549   | 0.089384    |
| 20            | 6             | 0           | 5.370917    | -1.861473   | 0.494830    |
| 21            | 6             | 0           | 5.647915    | -0.495253   | 0.396318    |
| 22            | 6             | 0           | 4.681646    | 0.377415    | -0.107177   |
| 23            | 6             | 0           | 0.677079    | 2.689230    | -0.491787   |
| 24            | 1             | 0           | -0.762955   | 2.395200    | 0.881109    |
| 25            | 1             | 0           | -2.239979   | 1.394879    | 2.750773    |
| 26            | 1             | 0           | -2.728426   | 1.357695    | 1.190639    |
| 27            | 1             | 0           | 0.858609    | 0.863150    | 1.915592    |
| 28            | 1             | 0           | -0.80945    | -0.338585   | 2.562889    |
| 29            | 1             | 0           | -1.841681   | -2.167000   | 1.209147    |
| 30            | 1             | 0           | -2.845105   | -1.425193   | 2.449485    |
| 31            | 1             | 0           | -2.599619   | -2.189624   | -1.115878   |
| 32            | 1             | 0           | -4.447644   | -1.855072   | -2.723629   |
| 33            | 1             | 0           | -6.434539   | -0.498403   | -2.082774   |
| 34            | 1             | 0           | -6.560717   | 0.491767    | 0.198847    |
| 35            | 1             | 0           | 2.271623    | 2.060221    | 0.725208    |
| 36            | 1             | 0           | 2.860058    | 1.658068    | -1.625166   |
| 37            | 1             | 0           | 1.688955    | 0.343604    | -1.729711   |
| 38            | 1             | 0           | 3.878427    | -3.404217   | 0.147937    |
| 39            | 1             | 0           | 6.117517    | -2.548370   | 0.882506    |
| 40            | 1             | 0           | 6.615342    | -0.110802   | 0.705693    |
| 41            | 1             | 0           | 4.901932    | 1.430959    | -0.190050   |
| 42            | 9             | 0           | 1.983244    | -1.944743   | -0.795745   |
| 43            | 1             | 0           | -4.727601   | 0.122233    | 1.814933    |

Rotational constants (GHZ): 0.4350130 0.1262131

0.1120536

### M1-N1

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X           | Y           | Z           |
| 1             | 8             | 0           | -0.601550   | -0.170235   | -0.674512   |
| 2             | 8             | 0           | -0.449536   | 3.017829    | 0.153133    |
| 3             | 8             | 0           | 1.025636    | 3.347843    | -1.459498   |
| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) | X       | Y       | Z       |
|---------------|---------------|-------------|-------------------------|---------|---------|---------|
| 1             | 8             | 0           | -0.971328               | 1.524173| -0.352061|
| 2             | 8             | 0           | 0.893901                | 3.853529| 0.241743 |
| 3             | 8             | 0           | 1.442380                | 3.225681| -1.852417|
| 4             | 7             | 0           | -2.486064               | 1.444581| 2.149922 |
| 5             | 7             | 0           | 0.836301                | 1.184777| 0.968989 |
| 6             | 6             | 0           | -1.371090               | 0.544051| 1.836474 |
| 7             | 6             | 0           | -1.882525               | -0.884460| 1.506396 |
| 8             | 6             | 0           | -2.895079               | -0.994953| 0.382733 |
| 9             | 6             | 0           | -2.498656               | -1.310419| -0.926684|
| 10            | 6             | 0           | -3.437753               | -1.423991| -1.953726|
| 11            | 6             | 0           | -4.795476               | -1.223006| -1.691581|

Rotational constants (GHz): 0.4350130 0.1262131

Standard basis: 6-31G(d) (6D, 7F)
Rotational constants (GHz):

| Center | Atomic Number | Atomic Type | X    | Y    | Z    |
|--------|---------------|-------------|------|------|------|
| 1      | 8             | 0           | -0.848551 | 1.419605 | -0.450801 |
| 2      | 8             | 0           | 1.955278  | 3.240229  | -1.724680 |
| 3      | 8             | 0           | 0.928894  | 3.854744  | 0.181879 |
| 4      | 7             | 0           | -2.449840 | 1.605720  | 2.018233 |
| 5      | 7             | 0           | 0.880005  | 1.165723  | 0.995130 |
| 6      | 6             | 0           | -1.378240 | 0.629540  | 1.787186 |
| 7      | 6             | 0           | -1.957336 | -0.784927 | 1.514010 |
| 8      | 6             | 0           | -2.975384 | -0.899940 | 0.395222 |
| 9      | 6             | 0           | -2.603404 | -1.326165 | -0.889612 |
| 10     | 6             | 0           | -3.550655 | -1.449900 | -1.908115 |
| 11     | 6             | 0           | -4.892508 | -1.147943 | -1.662205 |
| 12     | 6             | 0           | -5.278874 | -0.728252 | -0.387208 |
| 13     | 6             | 0           | -4.320920 | -0.610539 | 0.630484 |
| 14     | 6             | 0           | -0.431847 | 1.088656  | 0.671916 |
| 15     | 6             | 0           | 1.892422  | 1.623566  | 0.053538 |
| 16     | 6             | 0           | 2.232347  | 0.586551  | -1.043884 |
| 17     | 6             | 0           | 2.837019  | -0.677159 | -0.475601 |
| 18     | 6             | 0           | 2.062270  | -1.793082 | -0.159968 |
| 19     | 6             | 0           | 2.581893  | -2.967579 | 0.368202 |

Rotational constants (GHZ):

0.3224915
0.1645545

Standard basis: 6-31G(d) (6D, 7F)
| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|------------------------|
|               |               | X           | Y                       | Z                       |
| 1             | 8             | 0.927999    | 0.092384               | -1.533734               |
| 2             | 8             | 0.523477    | 2.490812               | 1.079129                |
| 3             | 8             | -0.718901   | 3.684232               | -0.381312               |
| 4             | 7             | 1.681617    | -2.427839              | -0.982420               |
| 5             | 7             | -0.580975   | 0.104207               | 0.182783                |
| 6             | 6             | 1.138081    | -1.610472              | 0.154059                |
| 7             | 6             | 2.263208    | -1.251952              | 1.155778                |
| 8             | 6             | 3.519292    | -0.650304              | 0.554481                |
| 9             | 6             | 3.623704    | 0.727140               | 0.306545                |
| 10            | 6             | 4.788786    | 1.263610               | -0.244030               |
| 11            | 6             | 5.868096    | 0.432942               | -0.557857               |
| 12            | 6             | 5.777018    | -0.938603              | -0.313069               |
| 13            | 6             | 4.612012    | -1.473517              | 0.241893                |
| 14            | 6             | 0.475613    | -0.382852              | -0.479304               |
| 15            | 6             | -1.220257   | 1.365316               | -0.183128               |
| 16            | 6             | -2.609905   | 1.477013               | 0.482126                |
| 17            | 6             | -3.587316   | 0.394043               | 0.087348                |
| 18            | 6             | -3.674299   | -0.805660              | 0.794460                |
| 19            | 6             | -4.553687   | -1.829853              | 0.472911                |
| 20            | 6             | -5.401392   | -1.656289              | -0.623177               |
| 21            | 6             | -5.346762   | -0.747699              | -1.363999               |
| 22            | 6             | -4.452339   | 0.536702               | 1.006949                |
| 23            | 6             | -0.376083   | 2.620021               | 0.203652                |
| 24            | 1             | 0.924480    | -2.893800              | -1.496281               |
| 25            | 1             | 2.337785    | -3.146366              | -0.655282               |
| 26            | 1             | 2.166708    | -1.804358              | -1.642752               |
| 27            | 1             | -0.854048   | -0.340800              | 1.052289                |
| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X           | Y           | Z           |
| 28            | 1             | 0           | 0.396446    | -2.229139   | 0.661079    |
| 29            | 1             | 0           | 1.817916    | -0.567095   | 1.884581    |
| 30            | 1             | 0           | 2.517300    | -2.173919   | 1.689577    |
| 31            | 1             | 0           | 2.791793    | 1.381670    | 0.550912    |
| 32            | 1             | 0           | 4.054671    | 2.333145    | -0.424819   |
| 33            | 1             | 0           | 6.774773    | 0.853094    | -0.944496   |
| 34            | 1             | 0           | 6.613060    | -1.592463   | -0.546022   |
| 35            | 1             | 0           | -1.341437   | 1.372110    | -1.269829   |
| 36            | 1             | 0           | -3.015126   | 2.450428    | 0.194350    |
| 37            | 1             | 0           | -2.475752   | 1.487965    | 1.570072    |
| 38            | 1             | 0           | -4.566332   | -2.734378   | 1.072386    |
| 39            | 1             | 0           | -6.098146   | -2.444317   | -0.893042   |
| 40            | 1             | 0           | -6.009002   | -0.332473   | -2.214764   |
| 41            | 1             | 0           | -4.419269   | 1.460461    | -1.579262   |
| 42            | 9             | 0           | -2.842675   | -0.986740   | 1.864505    |
| 43            | 1             | 0           | 4.552514    | -2.540634   | 0.445119    |

Rotational constants (GHZ): 0.4661365 0.1232890 0.1079489

M3

Center | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|-------|---------------|-------------|-------------------------|
|       |               |             | X           | Y           | Z           |
| 1     | 8             | 0           | -0.038382   | -1.056758   | 0.633286    |
| 2     | 8             | 0           | -0.486218   | 3.127443    | -1.245494   |
| 3     | 8             | 0           | 0.719044    | 3.973335    | 0.467015    |
| 4     | 7             | 0           | -1.185425   | -2.672946   | -1.079451   |
| 5     | 7             | 0           | 0.292949    | 0.650898    | -0.858270   |
| 6     | 6             | 0           | -1.064481   | -1.247702   | -1.535902   |
| 7     | 6             | 0           | -2.459918   | -0.615384   | -1.74265    |
| 8     | 6             | 0           | -3.286958   | -0.428072   | -0.48322    |
| 9     | 6             | 0           | -3.200514   | 0.762259    | 0.250267    |
| 10    | 6             | 0           | -3.953463   | 0.933049    | 1.413397    |
| 11    | 6             | 0           | -4.805090   | -0.083011   | 1.855289    |
| 12    | 6             | 0           | -4.903849   | -1.268872   | 1.124079    |
| 13    | 6             | 0           | -4.151753   | -1.437809   | -0.040898   |
| 14    | 6             | 0           | -0.209765   | -0.531910   | -0.478088   |
| 15    | 6             | 0           | 0.875130    | 1.621592    | 0.064881    |
| 16    | 6             | 0           | 2.423217    | 1.628417    | 0.027410    |
| 17    | 6             | 0           | 3.050818    | 0.317211    | 0.436806    |
| 18    | 6             | 0           | 3.476370    | -0.620410   | -0.505573   |
| 19    | 6             | 0           | 4.039288    | -1.845845   | -0.169294   |
| 20    | 6             | 0           | 4.185390    | -2.166480   | 1.181003    |
| 21    | 6             | 0           | 3.772783    | -1.257781   | 2.159799    |
| 22    | 6             | 0           | 3.214646    | -0.034672   | 1.785281    |
| 23    | 6             | 0           | 0.316108    | 3.036002    | -0.270238   |
| 24    | 1             | 0           | -0.285574   | -3.160468   | -1.157891   |
| 25    | 1             | 0           | -1.882205   | -3.185395   | -1.63280    |
| 26    | 1             | 0           | -1.454705   | -2.699438   | -0.087254   |
| 27    | 1             | 0           | -0.071402   | 1.082147    | -1.706109   |
| 28    | 1             | 0           | -0.542645   | -1.272980   | -2.493923   |
| 29    | 1             | 0           | -2.290193   | 0.350485    | -2.230397   |
| 30    | 1             | 0           | -2.94519    | -1.243800   | -2.469477   |
| 31    | 1             | 0           | -2.546987   | 1.559952    | -0.095065   |
| 32    | 1             | 0           | -3.878933   | 1.862503    | 1.971387    |
| 33    | 1             | 0           | -5.392911   | 0.051896    | 2.759065    |
| 34    | 1             | 0           | -5.570710   | -2.060437   | 1.454935    |
| 35    | 1             | 0           | 0.551136    | 1.362496    | 1.077716    |
| 36    | 1             | 0           | 2.749628    | 2.417923    | 0.709967    |
| Center | Atomic Number | Atomic Type | Coordinates (Angstroms) | X       | Y       | Z       |
|--------|---------------|-------------|-------------------------|---------|---------|---------|
| 37     | 1             | 0           | 2.750592                | 1.906068| -0.979545|
| 38     | 1             | 0           | 4.352728                | -2.523310| -0.957281|
| 39     | 1             | 0           | 4.622822                | -3.119689| 1.463247 |
| 40     | 1             | 0           | 3.888413                | -1.499939| 3.212245 |
| 41     | 1             | 0           | 2.898477                | 0.671851 | 2.543998 |
| 42     | 9             | 0           | 3.347255                | -0.322634| -1.827242|
| 43     | 1             | 0           | -4.244284               | -2.357478| -0.614664|

Rotational constants (GHz): 0.3475371 0.1560377 0.1335806

With water

M1a

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) | X     | Y     | Z     |
|---------------|---------------|-------------|-------------------------|-------|-------|-------|
| 1             | 8             | 0           | 0.813620                | 1.011972| 0.860443|
| 2             | 8             | 0           | -0.852977               | 3.650217| 0.541898|
| 3             | 8             | 0           | -2.159611               | 2.899450| 2.200513|
| 4             | 7             | 0           | 2.480690                | 1.707912| -1.272817|
| 5             | 7             | 0           | -0.873332               | 1.130318| -0.674285|
| 6             | 6             | 0           | 1.391131                | 0.693535| -1.454222|
| 7             | 6             | 0           | 1.945885                | -0.749146| -1.515166|
| 8             | 6             | 0           | 2.913123                | -1.160763| -0.425751|
| 9             | 6             | 0           | 2.470666                | -1.795514| 0.745018 |
| 10            | 6             | 0           | 3.377900                | -2.180580| 1.733493|
| 11            | 6             | 0           | 4.744124                | -1.935946| 1.570499|
| 12            | 6             | 0           | 5.198069                | -1.310011| 0.407809|
| 13            | 6             | 0           | 4.289007                | -0.930913| -0.582802|
| 14            | 6             | 0           | 0.404296                | 0.948046| -0.309009|
| 15            | 6             | 0           | -1.932818               | 1.483856| 0.270446|
| 16            | 6             | 0           | -2.344790               | 0.296681| 1.169718|
| 17            | 6             | 0           | -2.960558               | -0.853658| 0.407567|
| 18            | 6             | 0           | -2.199394               | -1.909973| -0.094183|
| 19            | 6             | 0           | -2.732185               | -2.978356| -0.803412|
| 20            | 6             | 0           | -4.108378               | -3.003898| -1.035924|
| 21            | 6             | 0           | -4.912983               | -1.967677| -0.554849|
| 22            | 6             | 0           | -4.340381               | -0.912493| 0.157630|
| 23            | 6             | 0           | -1.597576               | 2.778041| 1.084191|
| 24            | 1             | 0           | 2.049010                | 2.677205| -1.336895|
| 25            | 1             | 0           | 3.212596                | 1.600227| -1.982960|
| 26            | 1             | 0           | 2.912134                | 1.601265| -0.347488|
| 27            | 1             | 0           | -1.098336               | 1.107260| -1.660837|
| 28            | 1             | 0           | 0.925649                | 0.925279| -2.414113|
| 29            | 1             | 0           | 1.075965                | -1.413127| -1.530875|
| 30            | 1             | 0           | 2.440325                | -0.847538| -2.492278|
| 31            | 1             | 0           | 1.412102                | -1.995367| 0.879146 |
| 32            | 1             | 0           | 3.016650                | -2.675315| 2.631133|
| 33            | 1             | 0           | 5.449081                | -2.237608| 2.340320|
| 34            | 1             | 0           | 6.259200                | -1.123783| 0.265690|
| 35            | 1             | 0           | -2.794568               | 1.751259| -0.351512|
| 36            | 1             | 0           | -3.074095               | 0.680916| 1.885148 |
| 37            | 1             | 0           | -1.473907               | -0.039320| 1.739019 |
| 38            | 1             | 0           | -2.075252               | -3.766307| -1.157780|
| 39            | 1             | 0           | -4.545496               | -3.830940| -1.587576|
| 40            | 1             | 0           | -5.984968               | -1.983738| -0.728534|
| 41            | 1             | 0           | -4.970354               | -0.112027| 0.538153 |
| 42            | 8             | 0           | 1.013408                | 4.016880| -1.388140|
| 43            | 1             | 0           | 0.294154                | 3.801158| -0.731953|

S62
Rotational constants (GHz):  
|               |       |       |       |       |
|---------------|-------|-------|-------|-------|
|               | 0.2647566 | 0.1590607 | 0.1180401 |

Standard basis: 6-31G(d) (6D, 7F)

**M2b**

| Center Number | Atomic Number | Atomic Type | X (Angstroms) | Y (Angstroms) | Z (Angstroms) |
|---------------|---------------|-------------|---------------|---------------|---------------|
| 1             | 8             | 0           | -0.825648     | 0.097897      | 1.325708      |
| 2             | 8             | 0           | -0.285320     | 2.645811      | -0.986419     |
| 3             | 8             | 0           | 0.969275      | 3.707838      | 0.562635      |
| 4             | 7             | 0           | -1.502365     | -2.494615     | 0.420292      |
| 5             | 7             | 0           | 0.773111      | 0.184348      | -0.287586     |
| 6             | 6             | 0           | -0.978466     | -1.463814     | -0.537798     |
| 7             | 6             | 0           | -2.086395     | -0.985905     | -1.510707     |
| 8             | 6             | 0           | -3.352165     | -0.438188     | -0.882680     |
| 9             | 6             | 0           | -3.454101     | 0.909984      | -0.506954     |
| 10            | 6             | 0           | -4.621357     | 1.397417      | 0.083485      |
| 11            | 6             | 0           | -5.706402     | 0.545420      | 0.308823      |
| 12            | 6             | 0           | -5.620366     | -0.796735     | -0.070801     |
| 13            | 6             | 0           | -4.452730     | -1.281027     | -0.666865     |
| 14            | 6             | 0           | -0.337504     | -0.323344     | 0.260382      |
| 15            | 6             | 0           | 1.415070      | 1.394472      | 0.217880      |
| 16            | 6             | 0           | 2.839046      | 1.530076      | -0.365849     |
| 17            | 6             | 0           | 3.769718      | 0.387200      | -0.030103     |
| 18            | 6             | 0           | 3.854804      | -0.747803     | -0.837368     |
| 19            | 6             | 0           | 4.690414      | -1.823590     | -0.573444     |
| 20            | 6             | 0           | 5.494746      | -1.773818     | 0.567048      |
| 21            | 6             | 0           | 5.443171      | -0.658766     | 1.407454      |
| 22            | 6             | 0           | 4.591037      | 0.405798      | 1.106212      |
| 23            | 6             | 0           | 0.608109      | 2.694874      | -0.097171     |
| 24            | 1             | 0           | -0.726854     | -2.942239     | 0.922172      |
| 25            | 1             | 0           | -2.003365     | -3.230466     | -0.090992     |
| 26            | 1             | 0           | -2.154722     | -2.089058     | 1.142999      |
| 27            | 1             | 0           | 1.097476      | -0.199159     | -1.168695     |
| 28            | 1             | 0           | -0.212403     | -1.966635     | -1.129927     |
| 29            | 1             | 0           | -1.618271     | -0.230037     | -2.149778     |
| 30            | 1             | 0           | -2.331959     | -1.841897     | -2.148984     |
| 31            | 1             | 0           | -2.615374     | 1.579489      | -0.676275     |
| 32            | 1             | 0           | -4.684242     | 2.444757      | 0.366299      |
| 33            | 1             | 0           | -6.614395     | 0.926321      | 0.768106      |
| 34            | 1             | 0           | -6.462079     | -1.465119     | 0.088706      |
| 35            | 1             | 0           | 1.481686      | 1.305995      | 1.305818      |
| 36            | 1             | 0           | 3.251267      | 2.460139      | 0.033035      |
| 37            | 1             | 0           | 2.761561      | 1.647088      | -1.453119     |
| 38            | 1             | 0           | 4.703317      | -2.671957     | -1.250114     |
| 39            | 1             | 0           | 6.156959      | -2.604114     | 0.793719      |
| 40            | 1             | 0           | 6.069575      | -0.615021     | 2.293513      |
| 41            | 1             | 0           | 4.559019      | 1.275752      | 1.757404      |
| 42            | 8             | 0           | -3.003493     | -1.244968     | 2.443660      |
| 43            | 1             | 0           | -3.808336     | -0.949832     | 1.982616      |
| 44            | 1             | 0           | -2.346664     | -0.546123     | 2.229184      |
| 45            | 1             | 0           | -4.394842     | -2.324189     | -0.969731     |
| 46            | 9             | 0           | 3.064350      | -0.808662     | -1.952093     |
Rotational constants (GHz):

|                     | M3b    | M3c    |
|---------------------|--------|--------|
|                     | 0.4085334 | 0.3102529 |
|                     | 0.1152348 | 0.1493901 |
|                     | 0.1034024 | 0.1252192 |

**M3b**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms)   |
|---------------|---------------|-------------|---------------------------|
|               |               |             | X            | Y            | Z            |
| 1             | 8             | 0           | -0.047152    | -0.961496    | -0.477333    |
| 2             | 8             | 0           | 0.151942     | 3.413381     | 0.981744     |
| 3             | 8             | 0           | -1.037303    | 3.999069     | -0.847003    |
| 4             | 7             | 0           | 1.195214     | -2.333416    | 1.492207     |
| 5             | 7             | 0           | -0.450319    | 0.866626     | 0.826745     |
| 6             | 6             | 0           | 0.989024     | -0.863909    | 1.716100     |
| 7             | 6             | 0           | 2.337680     | -0.122069    | 1.883517     |
| 8             | 6             | 0           | 3.200494     | -0.019884    | 0.642315     |
| 9             | 6             | 0           | 3.025514     | 1.037398     | -0.263483    |
| 10            | 6             | 0           | 1.195214     | 3.413381     | 0.981744     |
| 11            | 6             | 0           | 1.195214     | -2.333416    | 1.492207     |
| 12            | 6             | 0           | -0.450319    | 0.866626     | 0.826745     |
| 13            | 6             | 0           | 0.989024     | -0.863909    | 1.716100     |
| 14            | 6             | 0           | 2.337680     | -0.122069    | 1.883517     |
| 15            | 6             | 0           | 3.200494     | -0.019884    | 0.642315     |
| 16            | 6             | 0           | 3.025514     | 1.037398     | -0.263483    |
| 17            | 6             | 0           | 1.195214     | 3.413381     | 0.981744     |
| 18            | 6             | 0           | 1.195214     | -2.333416    | 1.492207     |
| 19            | 6             | 0           | -0.450319    | 0.866626     | 0.826745     |
| 20            | 6             | 0           | 0.989024     | -0.863909    | 1.716100     |
| 21            | 6             | 0           | 2.337680     | -0.122069    | 1.883517     |
| 22            | 6             | 0           | 3.200494     | -0.019884    | 0.642315     |
| 23            | 6             | 0           | 3.025514     | 1.037398     | -0.263483    |
| 24            | 6             | 0           | 1.195214     | 3.413381     | 0.981744     |
| 25            | 6             | 0           | 1.195214     | -2.333416    | 1.492207     |
| 26            | 6             | 0           | -0.450319    | 0.866626     | 0.826745     |
| 27            | 6             | 0           | 0.989024     | -0.863909    | 1.716100     |
| 28            | 6             | 0           | 2.337680     | -0.122069    | 1.883517     |
| 29            | 6             | 0           | 3.200494     | -0.019884    | 0.642315     |
| 30            | 6             | 0           | 3.025514     | 1.037398     | -0.263483    |
| 31            | 6             | 0           | 1.195214     | 3.413381     | 0.981744     |
| 32            | 6             | 0           | 1.195214     | -2.333416    | 1.492207     |
| 33            | 6             | 0           | -0.450319    | 0.866626     | 0.826745     |
| 34            | 6             | 0           | 0.989024     | -0.863909    | 1.716100     |
| 35            | 6             | 0           | 2.337680     | -0.122069    | 1.883517     |
| 36            | 6             | 0           | 3.200494     | -0.019884    | 0.642315     |
| 37            | 6             | 0           | 3.025514     | 1.037398     | -0.263483    |
| 38            | 6             | 0           | 1.195214     | 3.413381     | 0.981744     |
| 39            | 6             | 0           | 1.195214     | -2.333416    | 1.492207     |
| 40            | 6             | 0           | -0.450319    | 0.866626     | 0.826745     |
| 41            | 6             | 0           | 0.989024     | -0.863909    | 1.716100     |
| 42            | 6             | 0           | 2.337680     | -0.122069    | 1.883517     |
| 43            | 6             | 0           | 3.200494     | -0.019884    | 0.642315     |
| 44            | 6             | 0           | 3.025514     | 1.037398     | -0.263483    |
| 45            | 6             | 0           | 1.195214     | 3.413381     | 0.981744     |
| 46            | 6             | 0           | 1.195214     | -2.333416    | 1.492207     |

Rotational constants (GHz):

|                     | 0.3102529 | 0.1493901 |
|                     | 0.1252192 |           |

**M3c**

S64
Center | Atomic Number | Atomic Number | Type | Coordinates (Angstroms) | X     | Y     | Z     |
|-------|---------------|---------------|------|------------------------|-------|-------|-------|
| 1     | 8             | 0             |      | -0.036794              | -0.794472 | 0.653528 |
| 2     | 8             | 0             |      | -0.668627              | 3.095475  | -1.801820 |
| 3     | 8             | 0             |      | 0.701558               | 4.189288  | -0.379631 |
| 4     | 7             | 0             |      | -1.264993              | -2.647490 | -0.756475 |
| 5     | 7             | 0             |      | 0.088951               | 0.711738  | -1.065111 |
| 6     | 6             | 0             |      | -1.257859              | -1.282059 | -1.367264 |
| 7     | 6             | 0             |      | -2.685114              | -0.704906 | -1.505460 |
| 8     | 6             | 0             |      | -3.380117              | -0.360970 | -0.203444 |
| 9     | 6             | 0             |      | -3.260089              | 0.924700  | 0.346879  |
| 10    | 6             | 0             |      | -3.889786              | 1.244876  | 1.551087  |
| 11    | 6             | 0             |      | -4.650687              | 0.284655  | 2.223249  |
| 12    | 6             | 0             |      | -4.782319              | -0.995917 | 1.681275  |
| 13    | 6             | 0             |      | -4.153423              | -1.314280 | 0.475289  |
| 14    | 6             | 0             |      | -0.332387              | -0.422079 | -0.493388 |
| 15    | 6             | 0             |      | 0.768336               | 1.793924  | -0.359232 |
| 16    | 6             | 0             |      | 2.311046               | 1.736169  | -0.496787 |
| 17    | 6             | 0             |      | 2.992136               | 0.670921  | 0.333814  |
| 18    | 6             | 0             |      | 3.170837               | -0.638379 | -0.112010 |
| 19    | 6             | 0             |      | 3.785448               | -1.636563 | 0.629345  |
| 20    | 6             | 0             |      | 4.264542               | -1.319145 | 1.901820  |
| 21    | 6             | 0             |      | 4.115143               | -0.020522 | 2.394036  |
| 22    | 6             | 0             |      | 3.489412               | 0.954953  | 1.615094  |
| 23    | 6             | 0             |      | 0.217417               | 3.150539  | -0.899007 |
| 24    | 1             | 0             |      | -0.319331              | -3.098532 | -0.892042 |
| 25    | 1             | 0             |      | -1.988573              | -3.238046 | -1.178732 |
| 26    | 1             | 0             |      | -1.440819              | -2.575692 | 0.252700  |
| 27    | 1             | 0             |      | -0.362592              | 1.027894  | -1.921583 |
| 28    | 1             | 0             |      | -0.829663              | -1.395446 | -2.365194 |
| 29    | 1             | 0             |      | -2.598601              | 0.190585  | -2.129039 |
| 30    | 1             | 0             |      | -3.275166              | -1.432294 | -2.075226 |
| 31    | 1             | 0             |      | -2.676064              | 1.677989  | -0.177166 |
| 32    | 1             | 0             |      | -3.790570              | 2.246354  | 1.961040  |
| 33    | 1             | 0             |      | -5.143587              | 0.535031  | 3.158662  |
| 34    | 1             | 0             |      | -5.379724              | -1.746138 | 2.192281  |
| 35    | 1             | 0             |      | 0.506908               | 1.733180  | 0.702520  |
| 36    | 1             | 0             |      | 2.687659               | 2.711463  | -0.177969 |
| 37    | 1             | 0             |      | 2.561730               | 1.615599  | -1.556394 |
| 38    | 1             | 0             |      | 3.875354               | -2.634863 | 0.212920  |
| 39    | 1             | 0             |      | 4.749814               | -2.084443 | 2.500192  |
| 40    | 1             | 0             |      | 4.488746               | 0.235045  | 3.381260  |
| 41    | 1             | 0             |      | 3.380475               | 1.965893  | 1.999881  |
| 42    | 0             | 0             |      | 1.302959               | -3.591251 | -1.202457 |
| 43    | 1             | 0             |      | 1.751279               | -2.734042 | -1.325762 |
| 44    | 9             | 0             |      | 2.700086               | -0.973068 | -1.357000 |
| 45    | 1             | 0             |      | 1.278209               | -3.970103 | -2.097999 |
| 46    | 1             | 0             |      | -4.271961              | -2.308846 | 0.051025  |

Rotational constants (GHZ): 0.2822911 0.1530634 0.1269860

Di F FF
Without water
M1

S65
| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|------------------------|
| 1             | 8             | 0           | 0.654056 1.523445 0.637119 |
| 2             | 8             | 0           | -1.244795 3.880275 -0.45070 |
| 3             | 8             | 0           | -2.441212 3.263888 1.743135 |
| 4             | 7             | 0           | 2.389311 1.817038 -1.472581 |
| 5             | 7             | 0           | -1.028203 1.240610 -0.888112 |
| 6             | 6             | 0           | 1.272317 0.811838 -1.568612 |
| 7             | 6             | 0           | 1.813932 -0.626394 1.381515 |
| 8             | 6             | 0           | 2.731352 -0.859557 -0.197396 |
| 9             | 6             | 0           | 2.277156 -1.376684 1.025114 |
| 10            | 6             | 0           | 3.157314 -1.619716 2.080871 |
| 11            | 6             | 0           | 4.520781 -1.351144 1.936806 |
| 12            | 6             | 0           | 5.005810 -0.836735 0.733232 |
| 13            | 6             | 0           | 4.101673 -0.608603 -0.293163 |
| 14            | 6             | 0           | 0.251670 1.226596 -0.499604 |
| 15            | 6             | 0           | -2.133909 1.635714 -0.010057 |
| 16            | 6             | 0           | -2.485378 0.541503 1.020566 |
| 17            | 6             | 0           | -3.068480 -0.706875 0.399275 |
| 18            | 6             | 0           | -2.280486 -1.795626 0.026421 |
| 19            | 6             | 0           | -2.781814 -2.950000 -0.560454 |
| 20            | 6             | 0           | -4.154673 -3.033612 -0.798397 |
| 21            | 6             | 0           | -4.986574 -1.968322 -0.443301 |
| 22            | 6             | 0           | -4.444511 -0.826147 0.148501 |
| 23            | 6             | 0           | -1.896016 3.051434 0.625361 |
| 24            | 1             | 0           | 2.120629 2.711559 -0.709243 |
| 25            | 1             | 0           | 3.246728 1.482081 -1.927991 |
| 26            | 1             | 0           | 2.592753 1.992829 -0.477725 |
| 27            | 1             | 0           | -1.235159 1.018189 -1.853906 |
| 28            | 1             | 0           | 0.855898 0.900946 -2.572052 |
| 29            | 1             | 0           | 0.941728 -1.280320 -1.304180 |
| 30            | 1             | 0           | 2.336444 -0.890970 -2.306042 |
| 31            | 1             | 0           | 1.221196 -1.598066 1.139762 |
| 32            | 1             | 0           | 2.777840 -2.023521 3.014610 |
| 33            | 1             | 0           | 5.208696 -1.540177 2.753556 |
| 34            | 1             | 0           | 6.057375 -0.616481 0.581689 |
| 35            | 1             | 0           | -2.994548 1.761540 -0.676284 |
| 36            | 1             | 0           | -3.219757 0.975454 1.701939 |
| 37            | 1             | 0           | -1.595274 0.302656 1.609570 |
| 38            | 1             | 0           | -2.103945 -3.757272 -0.818801 |
| 39            | 1             | 0           | -4.567960 -3.927272 -1.256607 |
| 40            | 1             | 0           | -6.056202 -2.028657 -0.621854 |
| 41            | 1             | 0           | -5.095776 -0.002177 0.430173 |
| 42            | 9             | 0           | 4.582541 -0.097311 -1.469675 |
| 43            | 9             | 0           | -0.934096 -1.732772 0.250028 |

Rotational constants (GHZ): 0.3108988 0.1439515 0.1163693

MI-CIP

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|------------------------|
| 1             | 8             | 0           | -0.594667 0.266888 -0.630677 |
| 2             | 8             | 0           | 0.065452 3.329119 -0.240300 |
| 3             | 8             | 0           | 1.742683 3.400938 -1.731600 |
| Center | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|--------|---------------|-------------|-------------------------|
|        |               |             | X          | Y          | Z          |
| 4      | 7             | 0           | -2.003266  | 2.106529  | 1.207586   |
| 5      | 7             | 0           | 0.953622   | 1.011546  | 0.886276   |
| 6      | 6             | 0           | -1.357230  | 0.790033  | 1.599362   |
| 7      | 6             | 0           | -2.365638  | -0.351435 | 1.800204   |
| 8      | 6             | 0           | -3.078198  | -0.934609 | 0.596445   |
| 9      | 6             | 0           | -2.730073  | -2.188470 | 0.073937   |
| 10     | 6             | 0           | -3.428525  | -2.751399 | -0.995710  |
| 11     | 6             | 0           | -4.504501  | -2.068342 | -1.567984  |
| 12     | 6             | 0           | -4.879054  | -0.818945 | 0.006416   |
| 13     | 6             | 0           | -4.159866  | -0.294752 | 0.081894   |
| 14     | 6             | 0           | 1.846945   | 1.662227  | 0.079164   |
| 15     | 6             | 0           | 2.486321   | 0.699470  | -1.102797  |
| 16     | 6             | 0           | 3.365726   | -0.355182 | -0.470928  |
| 17     | 6             | 0           | 2.888140   | -1.628668 | -0.155813  |
| 18     | 6             | 0           | 3.667143   | -2.617296 | 0.432856   |
| 19     | 6             | 0           | 4.999295   | -2.329306 | 0.733760   |

Rotational constants (GHZ): 0.3409395 0.1353588 0.1098685

**M1-N1**

| Center | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|--------|---------------|-------------|-------------------------|
|        |               |             | X          | Y          | Z          |
| 1      | 8             | 0           | 0.610788   | 1.524170  | 0.555266   |
| 2      | 8             | 0           | -1.228161  | 3.900659  | -0.171637  |
| 3      | 8             | 0           | -2.131806  | 3.278691  | 1.754962   |
| 4      | 7             | 0           | 2.250784   | 1.723596  | -1.765195  |
| 5      | 7             | 0           | -1.060022  | 1.228258  | -0.948215  |
| 6      | 6             | 0           | 1.232744   | 0.674262  | -1.626829  |
| 7      | 6             | 0           | 1.766916   | -0.758927 | -1.311421  |
| 8      | 6             | 0           | 2.738173   | -0.869165 | -0.158026  |
| 9      | 6             | 0           | 2.336248   | -1.218602 | 1.140496   |
| 10     | 6             | 0           | 3.255549   | -1.327748 | 2.185555   |
| 11     | 6             | 0           | 4.612460   | -1.088669 | 1.953827   |
| 12     | 6             | 0           | 5.047416   | -0.745666 | 0.672637   |

S67
| Center Number | Atomic Number | Atomic Type | X          | Y          | Z          |
|---------------|---------------|-------------|------------|------------|------------|
| 1             | 8             | 0           | 0.643390   | 1.637543   | 0.471781   |
| 2             | 8             | 0           | -1.317105  | 3.843540   | -0.314919  |
| 3             | 8             | 0           | -1.971249  | 3.240154   | 1.756135   |
| 4             | 7             | 0           | -2.336308  | 1.609687   | -1.903198  |
| 5             | 7             | 0           | -1.051003  | 1.168201   | -0.956666  |
| 6             | 6             | 0           | 1.240918   | 0.661967   | -1.67591   |
| 7             | 7             | 0           | 1.780283   | -0.751387  | -1.325202  |
| 8             | 6             | 0           | 2.731471   | -0.838795  | 0.149616   |
| 9             | 6             | 0           | 2.287364   | -1.060161  | 1.164094   |
| 10            | 6             | 0           | 3.180306   | -1.157581  | 2.232374   |
| 11            | 6             | 0           | 4.554687   | -1.039418  | 2.009686   |
| 12            | 6             | 0           | 5.030968   | -0.832579  | 0.714700   |
| 13            | 6             | 0           | 4.114399   | -0.739686  | -0.325823  |
| 14            | 6             | 0           | 0.258355   | 1.178341   | -0.616801  |
| 15            | 6             | 0           | -2.102131  | 1.600341   | -0.042166  |
| 16            | 6             | 0           | -2.464217  | 0.555614   | 1.035192   |
| 17            | 6             | 0           | -3.054564  | -0.704375  | 0.446218   |
| 18            | 6             | 0           | -2.274131  | -1.822790  | 0.154299   |
| 19            | 6             | 0           | -2.780289  | -2.993235  | -0.395825  |
| 20            | 6             | 0           | -4.145391  | -3.060252  | -0.678080  |
| 21            | 6             | 0           | -4.967572  | -1.964042  | 0.403170   |

Rotational constants (GHZ):

|   |   |   |
|---|---|---|
| M1-N2| 0.3098457 | 0.1439957 |

0.1178938
| Center | Atomic Number | Atomic Number | Atomic Type | Coordinates (Angstroms) | X       | Y       | Z       |
|--------|---------------|---------------|-------------|-------------------------|---------|---------|---------|
| 1      | 8             | 0             | 0           |                         | 0.528794| 1.560556| 0.541962|
| 2      | 8             | 0             | 0           |                         | -2.406828| 3.213723| 1.614120|
| 3      | 8             | 0             | 0           |                         | -1.354309| 3.853333| -0.270109|
| 4      | 7             | 0             | 0           |                         | 2.308776| 1.711733| -1.777258|
| 5      | 7             | 0             | 0           |                         | -1.090278| 1.142784| -0.989374|
| 6      | 6             | 0             | 0           |                         | 1.240237| 0.718359| -1.626933|
| 7      | 6             | 0             | 0           |                         | 1.818118| -0.688235| -1.308714|
| 8      | 6             | 0             | 0           |                         | 2.788811| -0.772141| -0.148918|
| 9      | 6             | 0             | 0           |                         | 2.374072| -1.013057| 1.170787|
| 10     | 6             | 0             | 0           |                         | 3.289121| -1.105150| 2.220747|
| 11     | 6             | 0             | 0           |                         | 4.656782| -0.961811| 1.973129|
| 12     | 6             | 0             | 0           |                         | 5.104465| -0.735419| 0.671244|
| 13     | 6             | 0             | 0           |                         | 4.166380| -0.648431| -0.350440|
| 14     | 6             | 0             | 0           |                         | 0.201658| 1.160965| -0.587995|
| 15     | 6             | 0             | 0           |                         | -2.183389| 1.569865| -0.126327|
| 16     | 6             | 0             | 0           |                         | -2.539266| 0.545657| 0.977606|
| 17     | 6             | 0             | 0           |                         | -3.038041| -0.764398| 0.411580|
| 18     | 6             | 0             | 0           |                         | -2.189629| -1.849437| 0.192692|
| 19     | 6             | 0             | 0           |                         | -2.612307| -3.064906| -0.329488|
| 20     | 6             | 0             | 0           |                         | -3.960160| -3.215577| -0.658794|
| 21     | 6             | 0             | 0           |                         | -4.84373| -2.155515| -0.457742|
| 22     | 6             | 0             | 0           |                         | -4.386986| -0.949708| 0.072543|
| 23     | 6             | 0             | 0           |                         | -1.903435| 2.988361| 0.387716|
| 24     | 1             | 0             | 0           |                         | -2.245030| 4.153961| 1.832533|
| 25     | 1             | 0             | 0           |                         | 2.723237| 1.862007| -0.856162|
| 26     | 1             | 0             | 0           |                         | 1.878547| 2.604425| -2.022839|
| 27     | 1             | 0             | 0           |                         | -1.312021| 0.834691| -1.927078|
| 28     | 1             | 0             | 0           |                         | 0.734248| 0.629462| -2.593207|
| 29     | 1             | 0             | 0           |                         | 0.978450| -1.365155| -1.123997|
| 30     | 1             | 0             | 0           |                         | 2.320735| -1.029179| -2.218197|

Rotational constants (GHZ): 0.3076817, 0.1440369, 0.1183687

M1-N3
| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|------------------------|
|               |               |             | X             | Y             | Z             |
| 1             | 8             | 0           | 0.718852      | 0.174322      | -1.534103     |
| 2             | 8             | 0           | 0.253813      | 2.548925      | 1.079395      |
| 3             | 8             | 0           | -1.040090     | 3.729960      | -0.346388     |
| 4             | 7             | 0           | 1.605706      | -2.283067     | -0.926110     |
| 5             | 7             | 0           | -0.793130     | 0.149274      | 0.180694      |
| 6             | 6             | 0           | 1.022259      | -1.468504     | 0.193973      |
| 7             | 6             | 0           | 2.129651      | -0.995659     | 1.16709      |
| 8             | 6             | 0           | 3.321752      | -0.318016     | 0.527209      |
| 9             | 6             | 0           | 3.410554      | 1.073014      | 0.368280      |
| 10            | 6             | 0           | 4.540742      | 1.665530      | -0.197830     |
| 11            | 6             | 0           | 5.614137      | 0.875880      | -0.618200     |
| 12            | 6             | 0           | 5.556236      | -0.511937     | -0.478556     |
| 13            | 6             | 0           | 4.417216      | -1.065721     | 0.086249      |
| 14            | 6             | 0           | 0.287781      | -0.297748     | -0.469132     |
| 15            | 6             | 0           | -1.465524     | 1.392242      | -0.188315     |
| 16            | 6             | 0           | -2.866131     | 1.462089      | 0.459060      |
| 17            | 6             | 0           | -3.799903     | 0.341028      | 0.065395      |
| 18            | 6             | 0           | -3.856271     | -0.850200     | 0.789940      |
| 19            | 6             | 0           | -4.695184     | -1.908756     | 0.471408      |
| 20            | 6             | 0           | -5.531165     | -1.781289     | -0.639998     |
| 21            | 6             | 0           | -5.507596     | -0.608061     | -1.398502     |
| 22            | 6             | 0           | -4.652205     | 0.437201      | -1.043811     |
| 23            | 6             | 0           | -0.653842     | 2.666718      | 0.215322      |
| 24            | 1             | 0           | 0.899537      | -2.901296     | -1.341561     |
| 25            | 1             | 0           | 2.397817      | -2.857831     | -0.615268     |
| 26            | 1             | 0           | 1.926945      | -1.636462     | -1.663114     |
| 27            | 1             | 0           | -1.033772     | -0.281566     | 1.066898      |
| 28            | 1             | 0           | 0.327794      | -2.113432     | 0.732894      |
| 29            | 1             | 0           | 1.652083      | -0.310378     | 1.872088      |
| 30            | 1             | 0           | 2.457552      | -1.871223     | 1.735112      |
| 31            | 1             | 0           | 2.577022      | 1.698995      | 0.692092      |
| 32            | 1             | 0           | 4.584119      | 2.744930      | -0.307570     |
| 33            | 1             | 0           | 6.495487      | 1.330404      | -1.056841     |
| 34            | 1             | 0           | 6.368064      | 1.154072      | -0.795484     |
| 35            | 1             | 0           | -1.572438     | 1.399190      | -1.276251     |
| 36            | 1             | 0           | 3.300066      | 2.418016      | 0.156431      |
| 37            | 1             | 0           | -2.746269     | 1.488743      | 1.548362      |
| 38            | 1             | 0           | -4.686349     | -2.803865     | 1.084952      |
| 39            | 1             | 0           | -6.193330     | -2.596861     | -0.907675     |

Rotational constants (GHz): 0.3082778 0.1430688 0.1168757

M2
| Center Number | Atomic Number | Atomic Type | X     | Y     | Z     |
|---------------|---------------|-------------|-------|-------|-------|
|               |               |             | 1     | 8     | 0     |
|               |               |             | -0.257070 | -0.984082 | 0.792847 |
|               |               |             | 2     | 8     | 0     |
|               |               |             | -0.137314 | 3.175517 | -1.332447 |
|               |               |             | 3     | 8     | 0     |
|               |               |             | 1.139375 | 4.041566 | 0.317703 |
|               |               |             | 4     | 7     | 0     |
|               |               |             | -1.147867 | -2.611383 | -0.650837 |
|               |               |             | 5     | 7     | 0     |
|               |               |             | 0.426923 | 0.687840 | -0.760388 |
|               |               |             | 6     | 6     | 0     |
|               |               |             | -0.932129 | -1.262931 | -1.287572 |
|               |               |             | 7     | 6     | 0     |
|               |               |             | -2.264986 | -0.555226 | -1.613618 |
|               |               |             | 8     | 6     | 0     |
|               |               |             | -3.109128 | -0.146672 | -0.423555 |
|               |               |             | 9     | 6     | 0     |
|               |               |             | -3.067150 | 1.151530 | 0.106904 |
|               |               |             | 10    | 6     | 0     |
|               |               |             | -3.870601 | 1.517257 | 1.188718 |
|               |               |             | 11    | 6     | 0     |
|               |               |             | -4.743577 | 0.589312 | 1.761493 |
|               |               |             | 12    | 6     | 0     |
|               |               |             | -4.811371 | -0.710143 | 1.254669 |
|               |               |             | 13    | 6     | 0     |
|               |               |             | -3.996065 | -1.036452 | 0.182406 |
|               |               |             | 14    | 6     | 0     |
|               |               |             | -0.019383 | -0.486542 | -0.313518 |
|               |               |             | 15    | 6     | 0     |
|               |               |             | 1.156832 | 1.667317 | 0.039527 |
|               |               |             | 16    | 6     | 0     |
|               |               |             | 2.692690 | 1.570562 | -0.147083 |
|               |               |             | 17    | 6     | 0     |
|               |               |             | 3.298237 | 0.265724 | 0.313163 |
|               |               |             | 18    | 6     | 0     |
|               |               |             | 3.495611 | -0.803876 | -0.562073 |
|               |               |             | 19    | 6     | 0     |
|               |               |             | 4.037729 | -2.022921 | -0.174539 |
|               |               |             | 20    | 6     | 0     |
|               |               |             | 4.402338 | -2.197888 | 1.161438 |
|               |               |             | 21    | 6     | 0     |
|               |               |             | 4.221511 | -1.154705 | 2.073716 |
|               |               |             | 22    | 6     | 0     |
|               |               |             | 3.677631 | 0.058273 | 1.647734 |
|               |               |             | 23    | 6     | 0     |
|               |               |             | 0.668867 | 3.091352 | -0.359429 |
|               |               |             | 24    | 1     | 0     |
|               |               |             | -0.701188 | -3.360761 | -1.188507 |
|               |               |             | 25    | 1     | 0     |
|               |               |             | -2.142947 | -2.843460 | -0.543624 |
|               |               |             | 26    | 1     | 0     |
|               |               |             | -0.706179 | -2.566700 | 0.288615 |
|               |               |             | 27    | 1     | 0     |
|               |               |             | 0.017758 | 1.094540 | -1.599590 |
|               |               |             | 28    | 1     | 0     |
|               |               |             | -0.393358 | -1.432341 | -2.221013 |
|               |               |             | 29    | 1     | 0     |
|               |               |             | -2.016940 | 0.334793 | -2.198601 |
|               |               |             | 30    | 1     | 0     |
|               |               |             | -2.831745 | -1.215585 | -2.278453 |
|               |               |             | 31    | 1     | 0     |
|               |               |             | -2.394781 | 1.878378 | -0.340914 |
|               |               |             | 32    | 1     | 0     |
|               |               |             | -3.818967 | 2.529109 | 1.579011 |
|               |               |             | 33    | 1     | 0     |
|               |               |             | -5.372001 | 0.870391 | 2.601168 |
|               |               |             | 34    | 1     | 0     |
|               |               |             | -5.477097 | -1.458372 | 1.671925 |
|               |               |             | 35    | 1     | 0     |
|               |               |             | 0.916207 | 1.502170 | 1.093919 |
|               |               |             | 36    | 1     | 0     |
|               |               |             | 3.127800 | 2.392858 | 0.427852 |
|               |               |             | 37    | 1     | 0     |
|               |               |             | 2.926137 | 1.744623 | -1.202692 |
|               |               |             | 38    | 1     | 0     |
|               |               |             | 4.166488 | -2.808711 | -0.912172 |
|               |               |             | 39    | 1     | 0     |
|               |               |             | 4.827377 | -3.144052 | 1.483432 |
|               |               |             | 40    | 1     | 0     |
|               |               |             | 4.507461 | -1.283637 | 3.113531 |
|               |               |             | 41    | 1     | 0     |
|               |               |             | 3.544202 | 0.870569 | 2.358149 |
|               |               |             | 42    | 9     | 0     |
|               |               |             | -4.057995 | -2.316787 | -0.306324 |
|               |               |             | 43    | 9     | 0     |
|               |               |             | 3.143883 | -0.650641 | -1.867342 |

Rotational constants (GHZ): 0.3286054 0.1421232 0.1182828

M3
With water

### M1a

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) | X    | Y    | Z     |
|---------------|---------------|-------------|-------------------------|------|------|-------|
| 1             | 8             | 0           |                         | 0.533817 | 1.017596 | 0.966793 |
| 2             | 8             | 0           |                         | -1.138182 | 3.646531 | 0.553211 |
| 3             | 8             | 0           |                         | -2.515438 | 2.895431 | 2.154203 |
| 4             | 7             | 0           |                         | 2.295965 | 1.755611 | -1.059328 |
| 5             | 7             | 0           |                         | -1.078558 | 1.127228 | -0.647557 |
| 6             | 6             | 0           |                         | 1.228883 | 0.733276 | -1.318214 |
| 7             | 6             | 0           |                         | 1.791902 | -0.706444 | -1.360897 |
| 8             | 6             | 0           |                         | 2.723121 | -1.106334 | -0.236120 |
| 9             | 6             | 0           |                         | 2.292499 | -1.807741 | 0.899697 |
| 10            | 6             | 0           |                         | 3.190070 | -2.187406 | 1.899126 |
| 11            | 6             | 0           |                         | 4.546628 | -1.873371 | 1.782644 |
| 12            | 6             | 0           |                         | 5.007783 | -1.179179 | 0.662752 |
| 13            | 6             | 0           |                         | 4.087358 | -0.818338 | -0.310561 |
| 14            | 6             | 0           |                         | 0.181322 | 0.962449 | -0.221641 |
| 15            | 6             | 0           |                         | 2.184803 | 1.469558 | 0.246247 |
| 16            | 6             | 0           |                         | 2.620759 | 0.280627 | 1.131761 |
| 17            | 6             | 0           |                         | -3.158438 | -0.892250 | 0.344859 |
| 18            | 6             | 0           |                         | -2.340501 | -1.935637 | -0.090049 |
| 19            | 6             | 0           |                         | -2.797741 | -3.024362 | -0.820502 |
| 20            | 6             | 0           |                         | -4.153742 | -3.085507 | 1.146405 |
| 21            | 6             | 0           |                         | -5.013395 | -2.063721 | 0.736467 |
| 22            | 6             | 0           |                         | -4.516064 | -0.987130 | 0.002065 |
| 23            | 6             | 0           |                         | -1.900780 | 2.772114 | 1.066085 |
| 24            | 1             | 0           |                         | 1.865044 | 2.718800 | 1.185577 |
| 25            | 1             | 0           |                         | 3.100051 | 1.632651 | 1.682882 |
| 26            | 1             | 0           |                         | 2.624416 | 1.678094 | 0.089133 |
| 27            | 1             | 0           |                         | -1.251050 | 1.126150 | -1.644769 |
| 28            | 1             | 0           |                         | 0.814975 | 0.970101 | -2.299358 |
| 29            | 1             | 0           |                         | 0.929878 | -1.378844 | -1.381685 |
| 30            | 1             | 0           |                         | 2.311003 | -0.816238 | -2.318062 |
| 31            | 1             | 0           |                         | 1.241179 | -2.061200 | 0.991091 |
| 32            | 1             | 0           |                         | 2.830029 | -2.733936 | 2.767205 |
| 33            | 1             | 0           |                         | 5.247763 | -2.167216 | 2.558004 |
| 34            | 1             | 0           |                         | 6.053890 | -0.920763 | 0.535101 |
| 35            | 1             | 0           |                         | -3.020906 | 1.721534 | -0.415604 |
| 36            | 1             | 0           |                         | -3.401945 | 0.651492 | 1.797811 |
| 37            | 1             | 0           |                         | -1.778376 | -0.028346 | 1.756402 |
| 38            | 1             | 0           |                         | -2.099871 | -3.800129 | -1.118977 |
| 39            | 1             | 0           |                         | -4.532322 | -3.928775 | 1.716500 |
| 40            | 1             | 0           |                         | -6.070275 | -2.107778 | -0.980882 |
| 41            | 1             | 0           |                         | -5.189350 | -0.198036 | 0.328206 |
| 42            | 8             | 0           |                         | 0.794073 | 4.031965 | -1.319125 |
| 43            | 1             | 0           |                         | 0.054971 | 3.810516 | -0.687978 |
| 44            | 9             | 0           |                         | 4.541246 | -0.138653 | -1.405910 |
| 45            | 9             | 0           |                         | -1.010476 | -1.893404 | 0.218699 |
| 46            | 1             | 0           |                         | 0.397888 | 3.902109 | -2.197184 |

Rotational constants (GHz):
- 0.2584356
- 0.1408309
- 0.1082277

### M2b
| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---------------|---------------|-------------|--------------------------|---|---|
|               | 1             | 8           | -0.613937                | 0.311449 | 1.372987 |
|               | 2             | 8           | -0.009169                | 2.622836 | -1.106031 |
|               | 3             | 8           | 1.298887                 | 3.762798 | 0.340172  |
|               | 4             | 7           | -1.475384                | -2.285296 | 0.580561 |
|               | 5             | 7           | 0.985049                 | 0.195933 | -0.238402 |
|               | 6             | 6           | -0.882225                | -1.325998 | -0.411874 |
|               | 7             | 6           | 1.953938                 | -0.784571 | -1.392560 |
|               | 8             | 6           | 3.193118                 | 1.187670 | -0.463420 |
|               | 9             | 6           | -4.456919                | 1.713954 | 0.103927  |
|               | 10            | 6           | -5.547878                | 0.882955 | 0.373149  |
|               | 11            | 6           | 5.248824                 | 0.699857 | -0.489583 |
|               | 12            | 6           | 0.151515                 | 0.202244 | 0.335237  |
|               | 13            | 6           | 1.674659                | 1.417474 | 0.166702  |
|               | 14            | 6           | 3.089647                | 1.466543 | 0.450321  |
|               | 15            | 6           | 3.987064                | 0.312781 | -0.065189 |
|               | 16            | 6           | 4.025175                | -0.639711 | 0.181421 |
|               | 17            | 6           | 4.829524                | -1.951463 | -0.504892 |
|               | 18            | 6           | 5.649417                | 1.869912 | 0.622608  |
|               | 19            | 6           | 5.643921                | -0.712662 | 1.405650 |
|               | 20            | 6           | 4.822724                | 0.362545 | 1.059601  |
|               | 21            | 6           | 0.199038                | 2.713373 | -0.234414 |
|               | 22            | 6           | -0.732102               | -2.797695 | 1.069204 |
|               | 23            | 1           | -2.092196               | -2.976491 | 0.010480 |
|               | 24            | 1           | -2.0642142              | -1.806062 | 1.315159 |
|               | 25            | 1           | 1.256907               | 0.243827 | -1.107965 |
|               | 26            | 1           | 1.665058               | 0.920606 | 1.351595 |
|               | 27            | 1           | -0.129050               | -1.900076 | -0.992908 |
|               | 28            | 1           | -1.146043               | -0.037416 | -2.012908 |
|               | 29            | 1           | -0.254085               | 1.631724 | -2.048623 |
|               | 30            | 1           | -0.254953               | 1.235416 | -0.873380 |
|               | 31            | 1           | -0.451049               | 2.773965 | 0.332934 |
|               | 32            | 1           | -6.453509               | 1.894949 | 0.813235  |
|               | 33            | 1           | -8.292445               | -1.154637 | 0.263719 |
|               | 34            | 1           | 1.175829               | 1.967637 | 1.257826 |
|               | 35            | 1           | 3.541992               | 2.403689 | 0.116634 |
|               | 36            | 1           | 2.993504               | 1.521248 | -1.540929 |
|               | 37            | 1           | 4.807188               | -2.832929 | -1.137562 |
|               | 38            | 1           | 6.354362               | 2.708662 | 0.884011 |
|               | 39            | 1           | 6.287764               | 1.287371 | 2.821238 |
|               | 40            | 1           | 4.826748               | 1.265189 | 1.665503 |
|               | 41            | 1           | -2.810230               | -0.871001 | 2.597500 |
|               | 42            | 1           | -3.615772               | -0.522313 | 2.174145 |
|               | 43            | 1           | -4.237770               | -2.303650 | -0.768408 |
|               | 44            | 1           | 3.218862               | -0.955535 | -1.915153 |
|               | 45            | 1           | -2.119599               | -0.220481 | 2.345279 |
|               | 46            | 1           | -2.119599               | -0.220481 | 2.345279 |

Rotational constants (GHz):

M3b

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---------------|---------------|-------------|--------------------------|---|---|
|               | 1             | 8           | -0.649118                | -0.012230 | -0.678241 |
|               | 2             | 8           | 2.916906                | 3.571117 | 0.496613  |

S73
| Center | Atomic Number | Atomic Type | X       | Y       | Z       |
|--------|--------------|-------------|---------|---------|---------|
| 1      | 8            |             | -0.058029 | -0.448410 | 0.694026 |
| 2      | 8            |             | 0.779051   | 3.483718  | -1.621485 |
| 3      | 8            |             | 1.999473   | 4.218554  | -0.067340 |
| 4      | 7            |             | -1.372783  | -1.993506 | -1.013365 |
| 5      | 7            |             | 0.570479   | 1.041644  | -0.929038 |
| 6      | 6            |             | -1.166335  | -0.573152 | -1.439729 |
| 7      | 6            |             | -2.494042  | 0.217214  | -1.483657 |
| 8      | 6            |             | -3.246332  | 0.305944  | -0.173965 |

Rotational constants (GHz): 0.2799775 0.1399500 0.1158776
| Center | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|--------|---------------|-------------|------------------------|
|        |               |             | X        | Y        | Z        |
| 1      | 8             | 0           | -0.485657 | -1.477381 | -1.065512 |
| 2      | 8             | 0           | -3.400895 | -2.371307 | -0.328264 |
| 3      | 8             | 0           | -4.572865 | -0.598671 | -1.119945 |
| 4      | 7             | 0           | 0.912732  | -3.343429 | 0.147370  |
| 5      | 7             | 0           | -1.532881 | -0.785942 | 0.859696  |
| 6      | 6             | 0           | 0.343835  | -2.292421 | 1.039126  |
| 7      | 6             | 0           | 1.476057  | -1.453299 | 1.646347  |
| 8      | 6             | 0           | 2.365914  | -0.827616 | 0.604836  |
| 9      | 6             | 0           | 2.043515  | 0.412450  | 0.034085  |
| 10     | 6             | 0           | 2.858661  | 0.964082  | -0.956795 |
| 11     | 6             | 0           | 3.996882  | 0.281186  | -1.395568 |

Rotational constants (GHz): 0.2561104 0.1355261 0.1144673

Cartesian Coordinates of Stationary Structures M1 and M1a at SMD(MP2/6-31G*)

FF M1

```markdown
| Center | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|--------|---------------|-------------|------------------------|
|        |               |             | X        | Y        | Z        |
| 1      | 8             | 0           | -0.485657 | -1.477381 | -1.065512 |
| 2      | 8             | 0           | -3.400895 | -2.371307 | -0.328264 |
| 3      | 8             | 0           | -4.572865 | -0.598671 | -1.119945 |
| 4      | 7             | 0           | 0.912732  | -3.343429 | 0.147370  |
| 5      | 7             | 0           | -1.532881 | -0.785942 | 0.859696  |
| 6      | 6             | 0           | 0.343835  | -2.292421 | 1.039126  |
| 7      | 6             | 0           | 1.476057  | -1.453299 | 1.646347  |
| 8      | 6             | 0           | 2.365914  | -0.827616 | 0.604836  |
| 9      | 6             | 0           | 2.043515  | 0.412450  | 0.034085  |
| 10     | 6             | 0           | 2.858661  | 0.964082  | -0.956795 |
| 11     | 6             | 0           | 3.996882  | 0.281186  | -1.395568 |
```
|   |   |   | X          | Y          | Z          |
|---|---|---|------------|------------|------------|
| 12 | 6 | 0 | 4.326887   | -0.952252  | -0.828845  |
| 13 | 6 | 0 | 3.514237   | -1.503257  | 0.165185   |
| 14 | 6 | 0 | -0.616877  | -1.479823  | 0.174614   |
| 15 | 6 | 0 | -2.673939  | -0.126445  | 0.233744   |
| 16 | 6 | 0 | -2.73416   | 1.008154   | -0.715375  |
| 17 | 6 | 0 | -1.263895  | 1.985736   | -0.165814  |
| 18 | 6 | 0 | -0.418175  | 2.662644   | -1.057720  |
| 19 | 6 | 0 | 0.502160   | 3.610184   | 0.602800   |
| 20 | 6 | 0 | 0.600344   | 3.889580   | 0.763017   |
| 21 | 6 | 0 | -1.169322  | 2.289222   | 1.200916   |
| 22 | 6 | 0 | -3.620141  | -1.134524  | -0.473428  |
| 23 | 6 | 0 | 1.663866   | -3.86355   | 0.616007   |
| 24 | 6 | 0 | 1.290897   | -2.910983  | -0.706894  |
| 25 | 6 | 0 | 1.587097   | -0.956549  | 1.860287   |
| 26 | 6 | 0 | -2.01136   | -2.809707  | 1.832786   |
| 27 | 6 | 0 | 1.012143   | -0.687916  | 2.277681   |
| 28 | 6 | 0 | 2.601166   | 1.928265   | -1.387497  |
| 29 | 6 | 0 | 4.629605   | 0.714368   | -2.166555  |
| 30 | 6 | 0 | 5.216621   | -1.484630  | -1.157034  |
| 31 | 6 | 0 | 3.783758   | -2.456411  | 0.619238   |
| 32 | 6 | 0 | 3.249855   | 0.299112   | 1.063193   |
| 33 | 6 | 0 | 3.196594   | 1.534515   | -0.902662  |
| 34 | 6 | 0 | -1.882906  | 0.580611   | -1.643581  |
| 35 | 6 | 0 | 0.174111   | 3.439984   | 2.726457   |
| 36 | 6 | 0 | 3.218414   | 4.619068   | 1.123730   |
| 37 | 6 | 0 | 1.142464   | 4.127492   | -1.314378  |
| 38 | 6 | 0 | 4.629605   | 0.714368   | -2.166555  |
| 39 | 6 | 0 | 5.216621   | -1.484630  | -1.157034  |
| 40 | 6 | 0 | 3.783758   | -2.456411  | 0.619238   |
| 41 | 6 | 0 | 3.249855   | 0.299112   | 1.063193   |
| 42 | 6 | 0 | 3.196594   | 1.534515   | -0.902662  |
| 43 | 6 | 0 | -1.882906  | 0.580611   | -1.643581  |

Rotational constants (GHz)

|             |   |   |             |
|-------------|---|---|-------------|
|             | 0.3230049 | 0.2377914 | 0.1613625  |

FF M1a

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|------------------------|
|               |               |             | X          | Y          | Z          |
| Center | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|--------|---------------|-------------|------------------------|
|        |               |             | X          | Y          | Z          |
| 1      | 8             | 0           | 0.246987  | -1.255560 | -1.004548  |
| 2      | 8             | 0           | -1.555925 | -3.592544 | -0.183036  |
| 3      | 8             | 0           | -3.496335 | -2.980601 | -1.185194  |
| 4      | 7             | 0           | 2.122516  | -2.582267 | 0.264396   |
| 5      | 7             | 0           | -1.115769 | -1.143943 | 0.845951   |
| 6      | 6             | 0           | 1.229902  | -1.747191 | 1.121393   |
| 7      | 6             | 0           | 1.982811  | -0.537296 | 1.683808   |
| 8      | 6             | 0           | 2.464453  | 0.429239  | 0.63970    |
| 9      | 6             | 0           | 1.720804  | 1.561032  | 0.276676   |
| 10     | 6             | 0           | 2.184004  | 2.447774  | -0.697661  |
| 11     | 6             | 0           | 3.412777  | 2.221759  | -1.324837  |
| 12     | 6             | 0           | 4.179462  | 1.105258  | -0.982807  |
| 13     | 6             | 0           | 3.684699  | 0.245884  | -0.012784  |
| 14     | 6             | 0           | 0.055283  | -1.367095 | 0.220183   |
| 15     | 6             | 0           | -2.379239 | -1.332885 | 0.129416   |
| 16     | 6             | 0           | -2.661137 | -0.253357 | -0.922700  |
| 17     | 6             | 0           | -2.574839 | 1.141384  | -0.365197  |
| 18     | 6             | 0           | -1.547582 | 2.009998  | -0.755622  |
| 19     | 6             | 0           | -1.469827 | 3.305822  | -0.233986  |
| 20     | 6             | 0           | -2.418163 | 3.746613  | 0.692046   |
| 21     | 6             | 0           | -3.447061 | 2.886362  | 1.090208   |
| 22     | 6             | 0           | -3.523794 | 1.595718  | 0.563861   |
| 23     | 6             | 0           | -2.469784 | -2.764424 | -0.471212  |
| 24     | 1             | 0           | 1.680871  | -3.492255 | 0.074082   |
| 25     | 1             | 0           | 3.035766  | -2.749135 | 0.704800   |
| 26     | 1             | 0           | 2.258389  | -2.119906 | -0.645867  |
Rotational constants (GHZ): 0.2989012 0.1996452 0.1344930

Mono1 F-FF M1a

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) | X     | Y     | Z     |
|---------------|---------------|-------------|-------------------------|-------|-------|-------|
| 1             | 8             | 0           |                         | 0.245121 | 1.149174 | 0.927735 |
| 2             | 8             | 0           |                         | -1.843212 | 3.410735 | 0.593819 |
| 3             | 8             | 0           |                         | -2.940318 | 2.382876 | 2.275673 |
| 4             | 7             | 0           |                         | 1.880621  | 1.955027 | -1.119465 |
| 5             | 7             | 0           |                         | -1.414450 | 0.955590 | -0.636543 |
| 6             | 6             | 0           |                         | 0.888460  | 0.871985 | -1.371552 |
| 7             | 6             | 0           |                         | 1.557380  | 0.958012 | -1.427319 |
| 8             | 6             | 0           |                         | 2.455368  | 0.818935 | -0.260531 |
| 9             | 6             | 0           |                         | 2.022971  | -1.564829| 0.845427  |
| 10            | 6             | 0           |                         | 2.883526  | -1.848906| 1.906190  |
| 11            | 6             | 0           |                         | 4.205124  | -1.393583| 1.879909  |
| 12            | 6             | 0           |                         | 4.668536  | -0.653063| 0.790343  |
| 13            | 6             | 0           |                         | 3.784067  | -0.393127| -0.246589 |
| 14            | 6             | 0           |                         | -0.135121 | 0.997778 | -0.251680 |
| 15            | 6             | 0           |                         | -2.518263 | 1.099759 | 0.303895  |
| 16            | 6             | 0           |                         | -2.692789 | -0.151735| 1.174142  |
| 17            | 6             | 0           |                         | -2.653785 | -1.415158| 0.355254  |
| 18            | 6             | 0           |                         | -1.689391 | -2.397691| 0.615152  |
| 19            | 6             | 0           |                         | -1.612911 | -3.556936| -0.163687 |
| 20            | 6             | 0           |                         | -2.506855 | -3.747600| -1.219905 |
| 21            | 6             | 0           |                         | -3.484793 | -2.781355| -1.479076 |
| 22            | 6             | 0           |                         | -3.555907 | -1.625068| -0.699270 |
| 23            | 6             | 0           |                         | -3.398931 | 2.401374 | 1.135304  |
| 24            | 1             | 0           |                         | 1.371544  | 2.872322 | -1.206323 |
| 25            | 1             | 0           |                         | 2.668240  | 1.913543 | -1.776690 |
| 26            | 1             | 0           |                         | 2.245188  | 1.878513 | -0.160837 |
| 27            | 1             | 0           |                         | -1.621190 | 0.838723 | -1.624192 |
| 28            | 1             | 0           |                         | 0.429919  | 1.088641 | -2.339644 |
| 29            | 1             | 0           |                         | 0.756087  | -1.253310| -1.485978 |
| 30            | 1             | 0           |                         | 2.126394  | -0.562948| -2.361768 |
| 31            | 1             | 0           |                         | 0.998610  | -1.926015| 0.856116  |
| 32            | 1             | 0           |                         | 2.525096  | -2.431398| 2.750833  |
| 33            | 1             | 0           |                         | 4.876849  | -1.612204| 2.704294  |
| 34            | 1             | 0           |                         | 5.690496  | -0.289882| 0.731893  |
| 35            | 1             | 0           |                         | -3.412688 | 1.221912 | -0.318474 |
Rotational constants (GHZ): 0.2550707 0.1730135 0.1286466

Mono2 F-FF M1

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X           | Y           | Z           |
| 1             | 8             | 0           | -0.965551   | 1.473094   | -0.341017   |
| 2             | 8             | 0           | 0.855430    | 3.837903   | 0.320806    |
| 3             | 8             | 0           | 1.536375    | 3.295661   | -1.772010   |
| 4             | 7             | 0           | -2.421699   | 1.401930   | 1.987778    |
| 5             | 7             | 0           | 0.891622    | 1.117655   | 0.948945    |
| 6             | 6             | 0           | -1.280163   | 0.453416   | 1.806334    |
| 7             | 6             | 0           | -1.815070   | -0.949863  | 1.481133    |
| 8             | 6             | 0           | -2.811336   | -1.003267  | 0.347828    |
| 9             | 6             | 0           | -2.401111   | -1.186958  | -0.981625   |
| 10            | 6             | 0           | -3.340719   | -1.228970  | -2.013065   |
| 11            | 6             | 0           | -4.702978   | -1.082792  | -1.734376   |
| 12            | 6             | 0           | -5.122382   | -0.906239  | -0.414033   |
| 13            | 6             | 0           | -4.182186   | -0.871957  | 0.619141    |
| 14            | 6             | 0           | -4.22104    | 1.053519   | 0.700957    |
| 15            | 6             | 0           | 1.833084    | 1.672738   | -0.020185   |
| 16            | 6             | 0           | 2.158588    | 0.659431   | -1.120664   |
| 17            | 6             | 0           | 2.824913    | -0.562164  | -0.553033   |
| 18            | 6             | 0           | 2.106520    | -1.697121  | -0.181888   |
| 19            | 6             | 0           | 2.679732    | -2.829852  | 0.380442    |
| 20            | 6             | 0           | 4.058721    | -2.833035  | 0.600145    |
| 21            | 6             | 0           | 4.823365    | -1.716581  | 0.248483    |
| 22            | 6             | 0           | 4.207943    | -0.598469  | -0.317867   |
| 23            | 6             | 0           | 1.341624    | 3.051901   | -0.544267   |
| 24            | 1             | 0           | -2.096793   | 2.298627   | 2.376159    |
| 25            | 1             | 0           | -3.134103   | 1.018361   | 2.624243    |
| 26            | 1             | 0           | -2.865291   | 1.594705   | 1.078749    |
| 27            | 1             | 0           | 1.245881    | 0.727529   | 1.817911    |
| 28            | 1             | 0           | -0.741439   | 0.425488   | 2.756272    |
| 29            | 1             | 0           | -0.947337   | -1.579896  | 1.268311    |
| 30            | 1             | 0           | -2.284307   | -1.332143  | 2.395933    |
| 31            | 1             | 0           | -1.345662   | -1.306100  | -1.207572   |
| 32            | 1             | 0           | -3.008166   | -1.376873  | -3.038004   |
| 33            | 1             | 0           | -5.432328   | -1.115491  | -2.540234   |
| 34            | 1             | 0           | -6.180662   | -0.804001  | -1.185275   |
| 35            | 1             | 0           | 2.750684    | 1.876410   | 0.546050    |
| 36            | 1             | 0           | 2.834287    | 1.138197   | -1.839277   |
| 37            | 1             | 0           | 1.240586    | 0.397714   | -1.655339   |
| 38            | 1             | 0           | 2.054087    | -3.680746  | 0.635299    |
| 39            | 1             | 0           | 4.530610    | -3.708285  | 1.038908    |
| 40            | 1             | 0           | 5.897618    | -1.717866  | 0.414093    |
| 41            | 1             | 0           | 4.805443    | 0.267949   | -0.597488   |
Rotational constants (GHz): 0.3325756
0.1694248
0.1358847

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Mono2 F-FF M1a

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X  | Y  | Z   |
| 1             | 8             | 0           | 0.885953 | 1.001910 | 0.764110 |
| 2             | 8             | 0           | -0.724174 | 3.600217 | 0.550321 |
| 3             | 8             | 0           | -1.584185 | 2.753995 | 2.456485 |
| 4             | 7             | 0           | 2.304617  | 1.513277 | -1.600219 |
| 5             | 7             | 0           | -0.942640 | 1.058801 | -0.604495 |
| 6             | 6             | 0           | 1.214184  | 0.494093 | -1.563061 |
| 7             | 6             | 0           | 1.788585  | -0.927715 | -1.512985 |
| 8             | 6             | 0           | 2.800834  | -1.175360 | -0.421549 |
| 9             | 6             | 0           | 2.422380  | -1.713526 | 0.817705  |
| 10            | 6             | 0           | 3.374399  | -1.940563 | 1.813053  |
| 11            | 6             | 0           | 4.718967  | -1.630862 | 1.587513  |
| 12            | 6             | 0           | 5.108022  | -1.102160 | 0.354712  |
| 13            | 6             | 0           | 4.155723  | -0.883029 | -0.644302 |
| 14            | 6             | 0           | 0.359940  | 0.862542  | -0.357913 |
| 15            | 6             | 0           | -1.865739 | 1.474375  | 0.448144  |
| 16            | 6             | 0           | -2.251632 | 0.292970  | 1.341500  |
| 17            | 6             | 0           | -2.892336 | -0.799600 | 0.533519  |
| 18            | 6             | 0           | -2.150094 | -1.846617 | -0.010290 |
| 19            | 6             | 0           | -2.689225 | -2.848987 | -0.805255 |
| 20            | 6             | 0           | -4.056034 | -2.803828 | -1.088770 |
| 21            | 6             | 0           | -4.843000 | -1.772176 | -0.568123 |
| 22            | 6             | 0           | -4.261810 | -0.784134 | 0.229559  |
| 23            | 6             | 0           | -1.322192 | 2.699036  | 1.224162  |
| 24            | 1             | 0           | 1.857303  | 2.460082  | -1.714335 |
| 25            | 1             | 0           | 2.954752  | 1.336779  | -2.377021 |
| 26            | 1             | 0           | 2.838544  | 1.495436  | -0.721516 |
| 27            | 1             | 0           | -1.278448 | 0.975560  | -1.559218 |
| 28            | 1             | 0           | 0.649566  | 0.618497  | -2.490866 |
| 29            | 1             | 0           | 0.939913  | -1.611483 | -1.416288 |
| 30            | 1             | 0           | 2.252635  | -1.116240 | -2.488844 |
| 31            | 1             | 0           | 1.379962  | -1.958304 | 1.000579  |
| 32            | 1             | 0           | 3.065831  | -2.362883 | 2.766707  |
| 33            | 1             | 0           | 5.458761  | -1.808316 | 2.364401  |
| 34            | 1             | 0           | 6.153535  | -0.870684 | 0.164721  |
| 35            | 1             | 0           | -2.767133 | 1.822763  | -0.075296 |
| 36            | 1             | 0           | -2.956789 | 0.650684  | 2.095964  |
| 37            | 1             | 0           | -1.361735 | -0.072307 | 1.861673  |
| 38            | 1             | 0           | -2.047516 | -3.637757 | -1.188053 |
| 39            | 1             | 0           | -4.501415 | -3.576693 | -1.709758 |
| 40            | 1             | 0           | -5.907755 | -1.737276 | -0.783843 |
| 41            | 1             | 0           | -4.876347 | 0.016702  | 0.637978  |
| 42            | 8             | 0           | 0.623240  | 3.703265  | -1.822934 |
| 43            | 1             | 0           | 0.078441  | 3.590234  | -0.997545 |
| 44            | 9             | 0           | -0.806241 | -1.903309 | 0.263996  |
| 45            | 1             | 0           | 0.046114  | 3.360605  | -2.528797 |
| 46            | 1             | 0           | 4.471600  | -0.496882 | -1.613184 |

Rotational constants (GHz): 0.2763970
0.1634400
0.1279857
### Di F-FF M1

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) | X     | Y     | Z     |
|---------------|---------------|-------------|-------------------------|-------|-------|-------|
| 1             | 8             | 0           | 0.662267                | 1.508437 | 0.484431 |
| 2             | 8             | 0           | -1.187671               | 0.833693 | -0.331070 |
| 3             | 8             | 0           | -1.960506               | 3.296459 | 1.729103 |
| 4             | 7             | 0           | 2.266111                | 1.516355 | -0.731089 |
| 5             | 7             | 0           | -1.100527               | 1.117904 | -0.924652 |
| 6             | 6             | 0           | 1.141069                | 0.533558 | -1.651007 |
| 7             | 6             | 0           | 1.681679                | -0.861781 | -1.301030 |
| 8             | 6             | 0           | 2.629903                | -0.97519 | -0.129841 |
| 9             | 6             | 0           | 2.217398                | -1.168405 | 1.183728 |
| 10            | 6             | 0           | 3.137801                | -1.208594 | 2.232888 |
| 11            | 6             | 0           | 4.496298                | -0.985023 | 1.990031 |
| 12            | 6             | 0           | 4.938881                | -0.715424 | 0.693677 |
| 13            | 6             | 0           | 3.959462                | -0.685033 | -0.322727 |
| 14            | 6             | 0           | 0.194808                | 1.091422 | -0.595409 |
| 15            | 6             | 0           | -2.115615               | 1.650297 | -0.019650 |
| 16            | 6             | 0           | -2.473870               | 0.639945 | 1.073042 |
| 17            | 6             | 0           | -3.042794               | -0.619607 | 0.483273 |
| 18            | 6             | 0           | -2.247866               | -1.725819 | 0.190878 |
| 19            | 6             | 0           | -2.724111               | -2.894661 | -0.387343 |
| 20            | 6             | 0           | -4.081629               | -2.967236 | -0.706770 |
| 21            | 6             | 0           | -4.920692               | -1.881827 | -0.436932 |
| 22            | 6             | 0           | -4.401301               | -0.725314 | 0.148351 |
| 23            | 6             | 0           | -1.696660               | 3.048111 | 0.515619 |
| 24            | 1             | 0           | 1.964711                | 2.382487 | -2.198857 |
| 25            | 1             | 0           | 3.073376                | 1.135640 | -2.242777 |
| 26            | 1             | 0           | 2.567215                | 1.761108 | -0.776927 |
| 27            | 1             | 0           | -1.381714               | 0.748028 | -1.828420 |
| 28            | 1             | 0           | 0.670744                | 0.505496 | -2.632632 |
| 29            | 1             | 0           | 0.817973                | -1.501209 | -1.102148 |
| 30            | 1             | 0           | 2.182526                | -1.257727 | -2.192808 |
| 31            | 1             | 0           | 1.165479                | -1.350991 | 1.377467 |
| 32            | 1             | 0           | 2.794381                | -1.422234 | 3.241582 |
| 33            | 1             | 0           | 5.213431                | -1.015858 | 2.806017 |
| 34            | 1             | 0           | 5.985959                | -0.540450 | 0.464336 |
| 35            | 1             | 0           | -3.004094               | 1.818217 | -0.642243 |
| 36            | 1             | 0           | -3.217766               | 1.098873 | 1.729258 |
| 37            | 1             | 0           | -1.585303               | 0.427705 | 1.674709 |
| 38            | 1             | 0           | -2.042680               | -3.719229 | -0.577087 |
| 39            | 1             | 0           | -4.479322               | -3.871695 | -1.159540 |
| 40            | 1             | 0           | -5.976808               | -1.937524 | -0.680123 |
| 41            | 1             | 0           | -5.057220               | 0.116576 | 0.364566 |
| 42            | 9             | 0           | 4.431033                | -0.414811 | -1.599239 |
| 43            | 9             | 0           | -0.912261               | -1.668215 | 0.504210 |

Rotational constants (GHZ): 0.3192068 0.1487963

### Di F-FF M1a

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) | X     | Y     | Z     |
|---------------|---------------|-------------|-------------------------|-------|-------|-------|
| 1             | 8             | 0           | 0.533455                | 1.033955 | 0.928082 |
| 2             | 8             | 0           | -1.115525               | 3.613404 | 0.507263 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 3 | 8 | 0 | -2.200267 | 2.806399 | 2.313633 |
| 4 | 7 | 0 | 2.193678 | 1.622787 | -1.209792 |
| 5 | 7 | 0 | -1.52683 | 1.059832 | -0.616927 |
| 6 | 6 | 0 | 1.112006 | 0.606832 | -0.36356 |
| 7 | 6 | 0 | 1.673579 | -0.821890 | -1.317607 |
| 8 | 6 | 0 | 2.645511 | -1.083837 | -0.197404 |
| 9 | 6 | 0 | 2.269387 | -1.650893 | 1.029208 |
| 10 | 6 | 0 | 3.212475 | -1.892587 | 2.029751 |
| 11 | 6 | 0 | 4.558566 | -1.577144 | 0.60970 |
| 12 | 6 | 0 | 4.965688 | -1.015593 | 0.33500 |
| 13 | 6 | 0 | 4.00367 | 0.910534 | -0.24420 |
| 14 | 6 | 0 | -2.185439 | 1.451058 | 0.415237 |
| 15 | 6 | 0 | -2.593925 | 0.276909 | 1.231609 |
| 16 | 6 | 0 | -3.099260 | -0.878094 | 0.195347 |
| 17 | 6 | 0 | -2.257165 | -1.906161 | -0.004903 |
| 18 | 6 | 0 | -2.667949 | -2.973821 | -0.791252 |
| 19 | 6 | 0 | -4.004130 | -3.020019 | -1.195347 |
| 20 | 6 | 0 | -4.887707 | -2.010266 | -0.802394 |
| 21 | 6 | 0 | -4.434299 | -0.954410 | -0.008718 |
| 22 | 6 | 0 | -1.776096 | 2.719055 | 1.128864 |
| 23 | 1 | 0 | 1.769500 | 2.568829 | -1.397601 |
| 24 | 1 | 0 | 2.978348 | 1.447171 | -1.849050 |
| 25 | 1 | 0 | 2.548762 | 1.609667 | -0.244311 |
| 27 | 1 | 0 | -1.378429 | 0.1016722 | -1.606368 |
| 28 | 1 | 0 | 0.657207 | 0.787003 | -0.34174 |
| 29 | 1 | 0 | 0.823199 | -1.505029 | -1.241166 |
| 30 | 1 | 0 | 2.163151 | -1.01239 | -2.278341 |
| 31 | 1 | 0 | 1.226009 | -1.904308 | 1.192032 |
| 32 | 1 | 0 | 2.897332 | -2.334903 | 2.971097 |
| 33 | 1 | 0 | 5.294022 | -1.764304 | 2.599626 |
| 34 | 1 | 0 | 6.002801 | -0.762948 | 0.409233 |
| 35 | 1 | 0 | -3.052499 | 1.739345 | -0.272431 |
| 36 | 1 | 0 | -3.383743 | 0.621924 | 1.903076 |
| 37 | 1 | 0 | -1.740905 | -0.022533 | 1.846431 |
| 38 | 1 | 0 | -1.954447 | -3.743311 | -1.072536 |
| 39 | 1 | 0 | -4.350440 | -3.846008 | -1.811073 |
| 40 | 1 | 0 | -5.928938 | -2.046804 | -1.12096 |
| 41 | 1 | 0 | -5.124603 | -0.171789 | 0.302324 |
| 42 | 8 | 0 | 0.559160 | 3.808164 | -1.653755 |
| 43 | 1 | 0 | -0.101796 | 3.65135 | -0.967081 |
| 44 | 9 | 0 | 4.399831 | -0.242169 | -1.555281 |
| 45 | 9 | 0 | -0.942647 | -1.872069 | 0.390280 |
| 46 | 1 | 0 | 0.100477 | 3.496004 | -2.454304 |

Rotational constants (GHz):

- 0.2658006
- 0.1445424
- 0.1149406

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