Supporting Information

for

Conformational preferences of fluorine-containing agrochemicals and their implications for lipophilicity prediction

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Additional linear correlation, main conformers from the Monte Carlo conformational search, Cartesian coordinates and energies of the conformers of agrochemicals I–VII and compounds 1–11 analyzed herein
Table of contents

**Figure S1:** Correlation between the experimental log $P$ of agrochemicals I–VII and predicted log $P$ (ACD/Labs).

Monte Carlo conformational search

Cartesian coordinates and energies of the conformers analyzed herein

**Figure S1:** Correlation between the experimental log $P$ of agrochemicals I–VII and predicted log $P$ (ACD/Labs).
Monte Carlo conformational search

**Table S1**: Structures, relative conformational energies referenced to the global energy minimum (in kcal mol\(^{-1}\)) and Boltzmann population (in %) of the main conformations (i.e., those with a population ≥5%) of agrochemicals I–VII obtained in the gas phase conformational search at the \(\omega\text{B97X-D}/6-31G(d,p)\) level of theory.

| Comp. | Conformation | \(\Delta E\) | Pop |
|-------|--------------|--------------|-----|
| I     | ![Image](image1) | 0.00         | 35  |
| I     | ![Image](image2) | 0.39         | 18  |
| I     | ![Image](image3) | 0.83         | 9   |
| I     | ![Image](image4) | 1.19         | 5   |
| II    | ![Image](image5) | 0.00         | 66  |
| II    | ![Image](image6) | 0.52         | 28  |
|  |  |  |  |
|---|---|---|---|
| II | 1.43 | 6 |
| III | 0.00 | 45 |
| III | 0.47 | 20 |
| III | 0.64 | 15 |
| III | 0.94 | 9 |
| III | 1.33 | 5 |
| IV | 0.00 | 39 |
| IV | 0.02 | 38 |
|   |   |   |
|---|---|---|
| IV | ![Molecule](image) | 0.74 | 11 |
| IV | ![Molecule](image) | 0.74 | 11 |
| V  | ![Molecule](image) | 0.00 | 43 |
| V  | ![Molecule](image) | 0.92 | 9  |
| V  | ![Molecule](image) | 1.01 | 8  |
| V  | ![Molecule](image) | 1.05 | 7  |
| V  | ![Molecule](image) | 1.15 | 6  |
| VI | ![Molecule](image) | 0.00 | 35 |
|    |    |    |    |    |    |    |    |
|----|----|----|----|----|----|----|----|
| VI |    | 0.07 | 31 |    |    |    |    |
| VI |    | 0.36 | 19 |    |    |    |    |
| VI |    | 1.12 | 5  |    |    |    |    |
| VII|    | 0.00 | 18 |    |    |    |    |
| VII|    | 0.03 | 17 |    |    |    |    |
| VII|    | 0.36 | 10 |    |    |    |    |
| VII|    | 0.38 | 9  |    |    |    |    |
| VII|    | 0.41 | 9  |    |    |    |    |
Cartesian coordinates and energies of the conformers analyzed herein

Cartesian coordinates (Å), energies (hartree), and the number of imaginary frequencies of the conformers of agrochemicals I–VII and compounds 1–11 analyzed herein at the ωB97X-D/6-311++G(d,p) level of theory.

Agrochem. Igg:

|     |     |     |     |
|-----|-----|-----|-----|
| C   | -1.24517900 | -1.80516000 | -0.83753500 |
| C   | -1.51138600 | -3.16716300 | -0.52113500 |
| C   | -2.73107400 | -3.42607700 | 0.04038300  |
| C   | -3.41500900 | -1.24521400 | 0.02691800  |
| C   | -0.60733100 | 0.10720100  | -1.37398100 |
| H   | -2.99047400 | -4.44746400 | 0.29202100  |
| O   | -4.23329000 | -0.23357800 | 0.26489100  |
| O   | -0.66546400 | -4.17563700 | -0.79861300 |
| N   | -3.67444000 | -2.47691700 | 0.30453600  |
| N   | -2.22382400 | -0.88635300 | -0.53665000 |
| N   | -1.80595900 | 0.36200200  | -0.86641700 |
| N   | -0.21436300 | -1.18116800 | -1.38491600 |
| C   | -5.50176400 | -0.57093700 | 0.83232500  |
| H   | -6.02370700 | 0.37686600  | 0.94018900  |
| H   | -6.05120400 | -1.23977000 | 0.16851600  |
| H   | -5.37037000 | -1.05374200 | 1.80191700  |
| C   | 0.73206900  | -3.93782300 | -0.59365000 |
| H   | 1.21348000  | -4.90491400 | -0.72856000 |
| H   | 1.12139900  | -3.21756400 | -1.31184500 |
| H   | 0.90822400  | -3.57157700 | 0.42301700  |
| N   | 0.20975800  | 1.14340000  | -1.80466300 |
| H   | -0.22559900 | 2.05329400  | -1.68516100 |
| S   | 1.80847600  | 1.19479100  | -1.24250500 |
| O   | 2.54033900  | 0.16452000  | -1.92029500 |
| O   | 2.19200200  | 2.57972800  | -1.32567800 |
|   |   |   |   |
|---|---|---|---|
| C | 1.59882600 | 0.68762600 | 0.49395100 |
| C | 0.56460900 | 1.31778000 | 1.20876100 |
| C | 2.29082000 | -0.37487300 | 1.09295100 |
| C | 0.13853500 | 0.80702600 | 2.43202700 |
| C | 1.87036300 | -0.85621100 | 2.32826600 |
| C | 0.78256800 | -0.28928700 | 2.97342500 |
| H | -0.68528200 | 1.26653800 | 2.96133700 |
| H | 2.40649200 | -1.67052700 | 2.79407100 |
| H | 0.45320000 | -0.69004600 | 3.92463400 |
| C | 3.54996400 | -1.02106300 | 0.51191000 |
| F | 4.38846200 | -0.11858600 | 0.01282800 |
| F | 3.28046800 | -0.85621100 | 2.32826600 |
| O | 0.02200900 | 2.41634900 | 0.64865600 |
| C | -1.24394400 | 2.86527300 | 1.07562000 |
| H | -1.98426600 | 3.24230300 | 2.10401100 |
| H | -1.64483800 | 3.81498900 | 0.35333100 |
| C | 0.82313800 | 1.97944300 | -0.81608400 |
| C | 0.83705500 | 3.36206100 | -0.47878000 |
| C | 2.00503200 | 3.84067400 | 0.04798100 |
| C | 3.09079700 | 1.83118200 | -0.03208200 |
| C | 0.54792700 | -0.01078500 | -1.37426700 |
| H | 2.07576400 | 4.88930700 | 0.31107700 |
| O | 4.09225000 | 0.99005800 | 0.15260500 |
| O | -0.19337000 | 4.19729900 | -0.70608500 |
| N | 3.12120300 | 3.08464400 | 0.26103100 |
| N | 1.96768300 | 1.26027600 | -0.56061800 |
| N | 1.78604300 | -0.03980400 | -0.90322800 |
| N | -0.08635600 | 1.17697300 | -1.34812800 |
| C | 5.30511800 | 1.55370000 | 0.65853100 |
| H | 5.99983100 | 0.71978500 | 0.72218200 |
| H | 5.68147900 | 2.31708800 | -0.02392400 |
| H | 5.13977800 | 1.99843500 | 1.64098900 |
| C | -1.51344200 | 3.69307600 | -0.47869500 |
| H | -2.17142400 | 4.55706000 | -0.54709700 |
| H | -1.78672700 | 2.94555600 | -1.22203200 |
| H | -1.58606000 | 3.25461500 | 0.52218000 |
| N | -0.06107300 | -1.18096300 | -1.80891000 |
| H | 0.54820900 | -1.98679200 | -1.71140700 |
| S | -1.61285100 | -1.55147500 | -1.23802000 |
| O | -2.38427800 | -0.06229000 | 1.06995600 |
| O | -2.54446200 | -0.70518500 | -1.92421600 |
| O | -1.70280200 | -2.98835400 | -1.30522300 |
| C | -1.50830100 | -0.98952700 | 0.48906500 |
| C | -0.37229900 | -1.39951300 | 1.20854900 |

Total energy = -2165.255461
Number of imaginary frequencies = 0

Agrochem. I\textsubscript{ag}:

|   |   |   |   |
|---|---|---|---|
| C | 0.82313800 | 1.97944300 | -0.81608400 |
| C | 0.83705500 | 3.36206100 | -0.47878000 |
| C | 2.00503200 | 3.84067400 | 0.04798100 |
| C | 3.09079700 | 1.83118200 | -0.03208200 |
| C | 0.54792700 | -0.01078500 | -1.37426700 |
| H | 2.07576400 | 4.88930700 | 0.31107700 |
| O | 4.09225000 | 0.99005800 | 0.15260500 |
| O | -0.19337000 | 4.19729900 | -0.70608500 |
| N | 3.12120300 | 3.08464400 | 0.26103100 |
| N | 1.96768300 | 1.26027600 | -0.56061800 |
| N | 1.78604300 | -0.03980400 | -0.90322800 |
| N | -0.08635600 | 1.17697300 | -1.34812800 |
| C | 5.30511800 | 1.55370000 | 0.65853100 |
| H | 5.99983100 | 0.71978500 | 0.72218200 |
| H | 5.68147900 | 2.31708800 | -0.02392400 |
| H | 5.13977800 | 1.99843500 | 1.64098900 |
| C | -1.51344200 | 3.69307600 | -0.47869500 |
| H | -2.17142400 | 4.55706000 | -0.54709700 |
| H | -1.78672700 | 2.94555600 | -1.22203200 |
| H | -1.58606000 | 3.25461500 | 0.52218000 |
| N | -0.06107300 | -1.18096300 | -1.80891000 |
| H | 0.54820900 | -1.98679200 | -1.71140700 |
| S | -1.61285100 | -1.55147500 | -1.23802000 |
| O | -2.38427800 | -0.06229000 | 1.06995600 |
|   |   |   |   |   |
|---|---|---|---|---|
| C | -0.03698800 | -0.78742100 | 2.41274100 |
| C | -2.05312100 | 0.51740700 | 2.28981000 |
| C | -0.87263400 | 0.18273600 | 2.93462800 |
| H | 0.86435400 | -1.07156600 | 2.93955600 |
| H | -2.73149600 | 1.22585500 | 1.46203400 |
| C | -3.74204600 | 0.32345300 | 0.49023000 |
| F | -4.40379100 | -0.73347600 | 0.02002300 |
| F | -3.66442700 | 1.25401400 | -0.46138400 |
| F | -4.52026500 | 0.85053700 | 0.57201400 |
| O | 0.35000700 | -2.39865900 | 0.66585000 |
| C | 1.67599600 | -2.63391400 | 1.08807700 |
| H | 2.29395200 | -1.74204700 | 0.94264800 |
| H | 1.71476500 | -2.97607100 | 2.12740800 |
| C | 2.18478300 | -3.74887700 | 0.19918800 |
| F | 3.45602000 | -4.04779900 | 0.57201400 |
| F | 2.21909000 | -3.33494400 | -1.09826700 |

Total energy = -2165.257772
Number of imaginary frequencies = 0

Agrochem. $I_{ga}$:

|   |   |   |   |   |
|---|---|---|---|---|
| C | -1.14331200 | -1.86663600 | -0.62430500 |
| C | -1.30695900 | -3.18075800 | -0.10623100 |
| C | -2.56637400 | -3.50436800 | 0.32115300 |
| C | -3.47120600 | -1.46679400 | -0.18111600 |
| C | -0.63617500 | 0.00583100 | -1.38774500 |
| H | -2.74990500 | -4.49478600 | 0.72022200 |
| O | -4.41658200 | -0.54807000 | -0.25323800 |
| O | -0.32662500 | -4.10124200 | -0.07064400 |
| N | -3.63666900 | -2.66192300 | 0.27463900 |
| N | -2.24854500 | -1.04821400 | -0.62342800 |
| N | -1.91884500 | 0.17822800 | -1.10560200 |
| N | -0.10971800 | -1.20392600 | -1.12358100 |
| C | -5.72070300 | -0.94368200 | 0.18242300 |
| H | -6.34479800 | -0.06594100 | 0.03459800 |
| H | -6.08263800 | -1.78152200 | -0.41501200 |
| H | -5.69975000 | -1.22153400 | 1.23453700 |
| C | 1.00760800 | -3.65206500 | 0.18895500 |
| H | 1.58498300 | -4.55618800 | 0.37151100 |
| H | 1.41481000 | -3.10515600 | -0.66023300 |
| H | 1.03107800 | -3.01370200 | 1.07855000 |
| N | 0.11310900 | 1.05746800 | -1.88673800 |
| H | -0.36680400 | 1.94740000 | -1.83604800 |
| S | 1.72676400 | 1.25182100 | -1.42580300 |
| O | 2.49045400 | 0.26760300 | -2.13388800 |
| O | 1.97355500 | 2.66380100 | -1.57445300 |
| C | 1.73723800 | 0.82413400 | 0.34281200 |
| C | 0.71620000 | 1.35879800 | 1.15153900 |
| C | 2.69866400 | -0.01637600 | 0.92665500 |
| C | 0.62959500 | 1.00653900 | 2.49667300 |
| C | 2.58689400 | -0.35783800 | 2.27022900 |
| C | 1.55164500 | 0.13888400 | 3.04239900 |

S8
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | -0.15416800 | 1.4199300 | 3.12089400 |
| H    | 3.32931200  | -1.00277600 | 2.71789900 |
| H    | 1.47947300  | -0.13289400 | 0.20701700 |
| C    | 3.92516200  | -0.57450000 | -0.47764300 |
| F    | 4.57794800  | 0.36395800  | -0.60222100 |
| F    | 3.63132000  | -1.59322200 | 0.20701700 |
| O    | -0.16072800 | 2.20497300  | 0.57096700  |
| H    | -1.33800600 | 2.55977700  | 1.26545500  |
| C    | 3.92516200  | -0.57450000 | 0.20701700 |
| F    | 4.57794800  | 0.36395800  | -0.60222100 |
| F    | 3.63132000  | -1.59322200 | 0.20701700 |
| O    | -0.16072800 | 2.20497300  | 0.57096700  |
| H    | -1.33800600 | 2.55977700  | 1.26545500  |
| H    | -1.12775600 | 3.30004600  | 2.04462900  |
| C    | -2.30576800 | 3.15144400  | 0.26118200  |
| H    | -2.59910800 | 2.44469100  | 0.60222100  |
| O    | -0.16072800 | 2.20497300  | 0.57096700  |
| H    | -1.33800600 | 2.55977700  | 1.26545500  |
| C    | -2.30576800 | 3.15144400  | 0.26118200  |
| H    | -2.59910800 | 2.44469100  | 0.60222100  |
| F    | -1.77438800 | 4.25721200  | -0.31854800 |
| F    | -3.41783400 | 3.53557800  | 0.95082500  |

Total energy = -2165.256929
Number of imaginary frequencies = 0

Agrochem. II:

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | -1.99701300 | 0.30844900 | 2.48681000 |
| C    | -2.33559000 | 0.31751200 | 1.13926000 |
| C    | -1.91355500 | -0.74228300 | 0.33340400 |
| C    | -1.22192800 | -1.79975800 | 0.97160800 |
| C    | -1.25215800 | -0.74358600 | 2.98181700 |
| H    | -2.31113400 | 1.10857300 | 3.14009500 |
| H    | -0.94985700 | -0.76145000 | 4.02414600 |
| N    | -0.87852700 | -1.78519500 | 2.24661100 |
| O    | -0.89252000 | -2.85644000 | 0.23385900 |
| C    | -0.00957100 | -3.82802700 | 0.80133000 |
| H    | -0.44342000 | -4.26468000 | 1.70071010 |
| H    | 0.11144800  | -4.58175200 | 0.02675200 |
| H    | 0.95179200  | -3.36712600 | 1.03250700 |
| S    | -2.11363800 | -0.83057400 | -1.46649500 |
| O    | -2.95919800 | -1.94735500 | -1.80318600 |
| O    | -2.37626900 | 0.49418200  | -1.93653800 |
| N    | -0.57955900 | -1.26970300 | -1.99781600 |
| H    | -0.48741700 | -2.27780200 | -2.00974800 |
| C    | 0.55027900  | -0.66296900 | -1.46069500 |
| C    | 2.48879300  | -0.49148000 | -0.69930900 |
| C    | 2.42224600  | 1.83487200  | -0.08770000 |
| C    | 3.69286800  | 1.67388700  | 0.39424200 |
| C    | 4.29619000  | 0.39695700  | 0.29079800 |
| H    | 4.21830600  | 2.50880500  | 0.83107900 |
| N    | 0.57093500  | 0.61246500  | -1.12764600 |
| N    | 1.66415800  | -1.38639800 | -1.22752200 |
| N    | 1.83553400  | 0.72916300  | -0.63467100 |
| N    | 3.73167700  | -0.66234500 | -0.24233600 |
| O    | 1.78031300  | 2.98154900  | 0.02413700 |
| O    | 5.53224400  | 0.30892200  | 0.77439900 |
| C    | 0.89189900  | 3.44400200  | -1.01795300 |
| H    | -0.05842100 | 2.91962800  | -0.97698300 |
| H    | 0.76857600  | 4.50569000  | -0.81769500 |
| H    | 1.35685600  | 3.29885000  | -1.99473400 |
### Agrochem. III:

|   |     |     |     |     |     |     |     |     |     |
|---|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| C | 6.19613300 | -0.95058400 | 0.66616600 |     |     |     |     |     |     |
| H | 7.17205500 | -0.79702100 | 1.12143500 |     |     |     |     |     |     |
| H | 5.64174400 | -1.72599200 | 1.19709500 |     |     |     |     |     |     |
| H | 6.30129000 | -1.24034300 | -0.38061100 |     |     |     |     |     |     |
| C | -3.17867300 | 1.49806600 | 0.65698600 |     |     |     |     |     |     |
| F | -2.45911000 | 2.39368100 | -0.02136700 |     |     |     |     |     |     |
| F | -4.21550100 | 1.10940700 | -0.08142800 |     |     |     |     |     |     |
| F | -3.69419000 | 2.15476500 | 1.71613000 |     |     |     |     |     |     |

**Total energy = -1943.511695**

**Number of imaginary frequencies = 0**
Total energy = -2187.404926
Number of imaginary frequencies = 0

**Agrochem. IV:**

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | 0.40797200| -2.08873100| -0.22931200|
| C    | 1.73450200| -2.47270100| -0.26280800|
| C    | 2.71274700| -1.49400600| -0.33171500|
| C    | 2.37302600| -0.13758200| -0.16955500|
| C    | 1.03431900| 0.21618800 | -0.08943200 |
| C    | 0.04118200| -0.75542000| -0.12647200|
| H    | 2.00830500| -3.51721200| -0.32800600 |
| H    | 0.73557100| 1.25216100 | -0.00153700|
| C    | 4.90012500| -1.00193000| 0.38131700 |
| H    | 5.91192300| 1.28495200 | 0.10272900 |
| N    | 3.41086800| 0.81774500 | -0.23755400|
| C    | 3.11655600| 2.21601700 | -0.52632700|
| H    | 4.04948700| 2.67549300 | -0.85525400|
| H    | 2.40119600| 2.26012100 | -1.35198600|
| C    | 2.59642400| 2.94712300 | 0.63143400 |
| C    | 2.16233700| 3.54069300 | 1.57799400 |
| H    | 1.78685700| 4.06775000 | 2.42246000 |
| C    | 4.70700100| 0.46530800 | 0.04315200 |
| O    | 5.62856800| 1.25023300 | 0.05397100 |
| O    | 4.01592600| -1.86359900| -0.31491300|
| H    | 4.77535500| -1.12796100| 1.46527100 |
| C    | -3.40694900| 0.45580600| -0.61470500|
| C    | -3.52704500| -0.13494600| 0.57494400 |
| C    | -4.50620400| 1.15486100| -1.33862200|
| C    | -4.78301700| -0.20739000| 1.37308500 |
| C    | -5.67066000| 1.41270900| -0.37221300|
| H    | -4.13025500| 2.08546800| -1.77499300|
| C    | -5.97740200| 0.18159800| 0.49035700 |
| H    | -4.90373400| -1.21026000| 1.79181800 |
| H    | -6.55946500| 1.71008600| -0.93379400|
| H    | -6.22795800| -0.66076700| -0.16467300|
| C    | -1.99417200| 0.32237100| -1.08298400|
| C    | -2.19972900| -0.69378600| 0.97674400 |
| O    | -1.50165600| 0.73934600| -2.09652800|
| O    | -1.90806700| -1.27576800| 1.98455000 |
| N    | -1.32122500| -0.38725600| -0.07655000|
| F    | -0.54232700| -3.02750700| -0.29621000|
| H    | -4.83124200| 0.53404600| -2.18205200|
| H    | -5.41196300| 2.25337500| 0.28204600 |
| H    | -6.85405600| 0.36837700| 1.11502500 |
| H    | -4.69803800| 0.46962900| 2.23164000 |

Total energy = -1243.183078
Number of imaginary frequencies = 0

**Agrochem. V:**

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | -1.96248800| 0.85130600| 0.38900900|
| C    | -3.25337300| 1.28372900| 0.10432200|
Total energy = -1939.678545
Number of imaginary frequencies = 0

Agrochem. VI:

C  -1.64910500  1.18403600  0.00066100
C  -0.28006900  1.32498500  -0.03516200
C   0.62311500  0.25562700  -0.26625800
C  -0.01765600  -0.99345900  -0.43968200
C  -1.38876600  -1.16826300  -0.32360000
C  -2.21324400  -0.07996000  -0.11751300
H  -2.26409900  2.06028800  0.16697800
Agrochem. VII:

\begin{align*}
\text{C} & \quad 1.72578800 \quad -1.18006000 \quad -0.16005700 \\
\text{C} & \quad 0.34575200 \quad -1.17613900 \quad -0.10002100 \\
\text{C} & \quad -0.44198700 \quad 0.00038600 \quad -0.00718300 \\
\text{C} & \quad 0.34341800 \quad 1.17994100 \quad 0.06957500 \\
\text{C} & \quad 1.72403800 \quad 1.18922900 \quad 0.10186700 \\
\text{C} & \quad 2.42973100 \quad 0.00601500 \quad -0.03853000 \\
\text{H} & \quad 2.24047700 \quad -2.12754300 \quad -0.25936300 \\
\text{H} & \quad 2.23740200 \quad 2.13917800 \quad 0.18210200 \\
\text{N} & \quad -0.25967000 \quad 2.52102800 \quad -0.01938300 \\
\text{O} & \quad 0.12174700 \quad 3.35588200 \quad 0.77597000 \\
\text{O} & \quad -1.05491400 \quad 2.72315700 \quad -0.91380400 \\
\text{N} & \quad -1.80367000 \quad -0.00095200 \quad 0.00428000 \\
\text{C} & \quad -2.56344400 \quad 0.97271600 \quad 0.79289600 \\
\text{H} & \quad -1.86076800 \quad 1.53139100 \quad 1.41366900 \\
\text{H} & \quad -3.05388900 \quad 1.69278900 \quad 0.13082500 \\
\text{C} & \quad -3.58022800 \quad 0.32759700 \quad 1.73477800 \\
\text{H} & \quad -4.12244300 \quad 1.15072000 \quad 2.21152300 \\
\text{H} & \quad -4.32722500 \quad -0.23282200 \quad 1.16470800 \\
\text{C} & \quad -2.94339700 \quad -0.56524400 \quad 2.79410800 \\
\end{align*}
S14

H  -2.22805600  0.00057000  3.39945300
H  -3.70143300 -0.96978400  3.46851900
H  -2.40871300 -1.40211000  2.34167300
C  -2.57599500 -0.97702000 -0.76905400
H  -3.04842400 -1.70043600 -0.09756600
H  -1.88437100 -1.53122500 -1.40211000
C  -3.61541400 -0.33501700 -1.68804000
H  -4.16573300 -1.15970600 -2.01254700
H  -4.35105900  0.22362100 -1.10178800
C  -3.00454500  0.55929200 -2.76129800
H  -2.30085000 -0.00483000 -3.38167300
H  -3.77817800  0.96132700 -3.41927200
C  -2.46262600  1.39777300 -2.32082200
C  -3.93010400  0.00208200  0.00032900
F  -4.44289700  1.14437400 -0.48056700
F  -4.44168900 -1.00837000 -0.71760000
F  -3.93010400 -0.13619400  1.25608300
N  -0.25060200 -2.51964000 -0.00565000
O   0.12183300 -3.35139000 -0.80845600
O  -1.03117300 -2.72676500  0.90058800

Total energy = \(-1269.472161\)
Number of imaginary frequencies = 0

Comp. 1:

C  -0.06226700  0.00000000  0.35560500
C   1.37160000  0.00000000 -0.09411100
F  -0.71266300  1.09740300 -0.13533600
H   1.87578700  0.88888300  0.29241000
H   1.87578700 -0.88888300  0.29241000
H   1.41672800  0.00000000 -1.18103200
H  -0.19636500  0.00000000  1.44110600
F  -0.71266300 -1.09740300 -0.13533600

Total energy = \(-278.318378\)
Number of imaginary frequencies = 0

Comp. 2:

C  -0.40834800  0.00393500  0.00000000
C   0.92205600  0.73661000  0.00000000
F  -0.55605100 -0.76852800 -1.07955600
H   0.98127800  1.35531700 -0.89749500
H   0.98127800  1.35531700  0.89749400
F  -0.55605100 -0.76852800  1.07955600
F  -1.40031900  0.91002600  0.00000000
F    1.95188700 -0.16784900  0.00000000

Total energy = \(-476.803130\)
Number of imaginary frequencies = 0

Comp. 3:

C   0.77708800 -0.00001000  0.00000000
Total energy = -675.296225  
Number of imaginary frequencies = 0 

Comp. 4:

C  -0.34421300  -0.06048500  0.00000000  
C  -1.07312800  1.25416000  0.00000000  
F  -0.67344000  -0.79493900  1.08136200  
F  -0.67344000  -0.79493900  -1.08136200  
H  -0.80728100  1.82234200  -0.89044500  
H  -0.80728100  1.82234200  -1.08136200  
Cl  1.43448200  -0.14411100  0.00000000  

Total energy = -737.926067  
Number of imaginary frequencies = 0 

Comp. 5:

C  -0.45338100  0.45829600  0.00000000  
C  0.94633500  -0.22390600  0.00000000  
F  -0.54693400  1.23314600  1.08198200  
F  -0.54693400  1.23314600  -1.08198200  
Cl  -1.75388200  -0.73107400  0.00000000  
F  1.88757200  0.71519500  0.00000000  
F  1.09527400  -0.97841500  1.08192300  
F  1.09527400  -0.97841500  -1.08192300  

Total energy = -1035.646536  
Number of imaginary frequencies = 0 

Comp. 6:

C  0.00000000  0.32606700  0.08926300  
C  0.00000000  1.50736400  -0.84806600  
F  0.00000000  0.75612100  1.37244700  
Cl  -1.46110000  -0.68195900  -0.13519000  
H  -0.89190800  2.10680300  -0.66001400  
H  0.00000100  1.16732400  -1.88272800  
H  0.89190800  2.10680400  -0.66001300  
Cl  1.46110000  -0.68195900  -0.13519000  

Total energy = -1098.277782  
Number of imaginary frequencies = 0 

Comp. 7a:
Total energy = -1395.996957
Number of imaginary frequencies = 0

Comp. 7g:

C  -0.12062700  0.77196600  0.32737500
C   0.12062700 -0.77196600  0.32737500
F   1.05645100  1.39705900  0.35328300
Cl  -1.05645100  1.30308500 -1.06907400
Cl   1.05645100 -1.30308500 -1.06907400
F   -0.77863800  1.07927300  1.44783000
F   -1.05645100 -1.39705900 -1.08211700
F    0.77863800 -1.07927300  1.44783000

Total energy = -1395.996642
Number of imaginary frequencies = 0

Comp. 8:

C   0.41828500  0.00000000  0.30745800
C  -1.08525300  0.00000000 -0.10702300
Cl  1.21101300  1.45870600 -0.29764100
F   0.46198800  0.00000000  1.64860400
F  -1.21624300 -0.00000000 -1.42758400
F  -1.68801800  1.07757000  0.38489100
F  -1.68801800  1.07756900 -0.38489100
Cl  1.21101300  1.45870600 -0.29764100

Total energy = -1395.999748
Number of imaginary frequencies = 0

Comp. 9a:

C   0.68276600  0.00004000  0.27518000
C  -0.87818400 -0.00014800  0.41809800
Cl  1.23677400  1.45955500 -0.55269100
F   1.17532800 -0.00002400  1.52426300
F  -1.23469500  1.07736100  1.11998000
F  -1.23450100 -1.07787000  1.11979100
Cl  1.23707100 -1.45931100 -0.55300100
Cl  -1.71988500  0.00007600  1.13171800

Total energy = -1756.349318
Number of imaginary frequencies = 0
Comp. 9g:

C | 0.58143400 | 0.14781200 | 0.30903900
C | -0.72840100 | -0.53085400 | -0.21650600
Cl | 0.77953000 | 1.76002000 | -0.38623100
F | 0.48716100 | 0.24862600 | 1.64172200
F | -0.82296400 | -1.74515800 | 0.32811000
F | -0.66561800 | -0.66952600 | -1.53984200
Cl | 1.96961100 | -0.87878100 | -0.08900200
Cl | 1.96910700 | 0.40068900 | 0.21493200

Total energy = -1756.349596
Number of imaginary frequencies = 0

Comp. 10g:

C | -0.72179700 | -0.00008000 | 0.31161300
C | 0.72175200 | 0.00004900 | -0.31140700
Cl | -1.61055300 | -1.44903900 | -0.18925100
F | -0.60859200 | 0.00005500 | 1.64519100
F | 0.60819300 | 0.00019000 | -1.64499400
Cl | -1.61089800 | 1.44885900 | 1.18905300
Cl | 1.61077100 | 1.44907400 | 0.18886100
Cl | 1.61090800 | -1.44877700 | 0.18926600

Total energy = -2116.701562
Number of imaginary frequencies = 0

Comp. 10s:

C | 0.72021100 | 0.31626700 | -0.25663600
C | -0.72021100 | -0.31626700 | -0.25663500
Cl | 1.94620600 | -0.96047400 | -0.33875900
F | 0.82211500 | 1.06325400 | -1.36650500
F | -0.82211700 | -1.06325400 | -1.36650500
Cl | 0.98296700 | 1.34909900 | 1.15277900
Cl | -0.98296700 | -1.34909900 | 1.15278000
Cl | -1.94620500 | 0.96047500 | -0.33875800

Total energy = -2116.701671
Number of imaginary frequencies = 0

Comp. 11:

C | 0.00000000 | 0.06553200 | 0.00000000
C | -0.00062500 | 1.38020000 | 0.00000000
H | -0.93837200 | 1.91398100 | 0.00000000
H | 0.93685800 | 1.91451200 | 0.00000000
F | -1.07598400 | -0.69510500 | 0.00000000
F | 1.07657000 | -0.69410500 | 0.00000000

Total energy = -277.068945
Number of imaginary frequencies = 0